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Combining circularity and environmental metrics to assess material flows of PV silicon

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Abstract. A product made from virgin raw materials that ends up in a landfill presents a linear supply chain model. Today's photovoltaic (PV) industry is still largely based on this model. With the increasing volume of production, the raw materials required for it, and consequently the volume of waste, the application of circular economy principles in the PV sector can significantly increase its environmental efficiency. This study analyzes the impact of circularity on the supply chain of PV silicon used for PV module production. Four scenarios based on the combination of technological pathways and circularity options are created. Their evaluation is carried out by the methodologies of Material Circularity Indicator (MCI) and Life Cycle Assessment (LCA). The State-of-art case of the PV polysilicon supply chain corresponds to the MCI score of 0.54. Closed-loop circularity solutions provide the MCI score of 0.80 presenting the potential for a circular economy approach in the industry. LCA results show the reduction of environmental impact by 12% with improved circularity. The study presents the benefits of potential circularity options within the supply chain as well as the impact of technological development on the polysilicon demand.

Keywords: Circularity / life cycle assessment / photovoltaics / polysilicon / metrics

1 Introduction

In 2021, the cumulative photovoltaic (PV) installed capacity reached more than 950 GWp [1]. To meet long-term climate goals, an increase of PV installations is projected by energy system models [2–4]. 100% renewable electricity scenarios designed under the LUT Energy System Transition Model showed the following: global PV installed capacity should reach 7.1–9.1 TWp for 2030 [2], the PV installed capacity in Europe should reach 1.7–2.0 TWp for 2050 [3]. Goldschmidt et al. assessed PV deployment up to 2100 to limit climate change to 1.5 °C with the REMIND model. The installed PV capacity would reach 80–170 TWp until 2100 depending on the conditions for PV deployment [4]. To achieve extensive PV deployment, the quantity of required materials is high [5]. Possible options to meet this demand are to use virgin materials or to implement circular economy (CE) approaches to the industry. A product made from virgin raw materials that ends up in a landfill presents a linear supply chain model. Today's photovoltaic industry is still largely based on this model [6]. Closing the loops within production steps and after the product's lifetime is a way to implement CE principles. The main purpose of circularity is to retain the highest value of materials restoratively. Depending on the chosen waste treatment pathway, the PV modules end up in landfills or are reused or recycled as parts or materials for new products [6]. Today's material demand for the PV industry cannot be covered by the amount of generated waste [7]. As solar panels have a long service life, their End-of-life (EOL) treatment was not a concern during their first years of development. PV lifetime estimates are generally based on manufacturers' warranty of at least 80% power output after 25 years of operation [8]. Tan et al. estimated practical lifetimes for PV in Australia of 15–20 years. They concluded that practical lifetimes are highly dependent on a variety of country-specific technical, economic, and social factors [9]. The worldwide second-hand (re-used) photovoltaics market size is estimated to be around 500–1000 MWp/year [10,11]. Using these modules in high-income countries could be interesting to repair PV systems that still receive feed-in tariff. For developing regions, second-hand modules are well adapted to build new small to medium size PV systems that are often off-grid. However, the lack of legislation and recycling facilities remains challenging to-date and poses a risk for final disposal in these regions [11]. With the expected increasing production volume, the required raw materials, and the associated amount of waste, the application of circular economy principles in the PV sector becomes a critical topic.

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Table 1. Technical details related to functional unit.

Parameter	Value	Unit
Power	1	kWp
Irradiation (global average) [22]	1690	$kWh/m^2/y$
Performance ratio [23]	0.75	kWh/kWp
Yearly PV energy production (first year)	1271	kWh
Average module service time	25	Years
Degradation	0.5	%/annual
PV energy production (25 years)	30.0	MWh
PV energy production (35 years)	40.9	MWh

The application of circular economy approaches has been discussed in terms of environmental, technological, economic, and legislative arguments [7,12–14]. However, a research gap has been identified in the quantitative assessment of circularity in PV. A circular model is based on three principles: design out waste and pollution, keep products and materials in use, and regenerate natural systems [15]. As these principles are represented by various parameters the need for universal metric remains. A circularity metric provides a chance to estimate various CE scenarios also to combine the results with other indicators. The Material Circularity Indicator allows stakeholders to understand how far the products are on transitioning from a linear to a circular supply chain. The MCI of a product ranges, by convention, from 0.1 (fully linear) to 1 (fully circular) [15]. More circularity on material flows does not necessarily lead to more environmentally friendly solutions. The interaction between circularity and life-cycle-based environmental indicators has been discussed in the literature [16–18]. The aforementioned studies present the results comparing different scenarios in terms of circularity metrics and selected environmental impact categories for alkaline batteries, used tires, and beer packaging. Schulte et al. integrated CE metric to Life Cycle Assessment (LCA) and submitted upgraded results on environmental impacts [19]. Mantalovas and Di Mino created the methodology for the so-called Environmental Sustainability and Circularity Indicator (ESC_i), which combines the MCI and LCA results to one unitless score [20]. Still, there is no widely accepted universal metric combining circularity and environmental performances.

So far, the circularity in the PV sector, both for the module as a whole and its materials, has not been assessed through the dedicated circularity indicators. Implementing these indicators in the field allows stakeholders to evaluate how CE strategies contribute to a reduced material consumption and more circular flows. The integration of circularity and environmental indicators has not yet been investigated for silicon. Silicon is the most common semiconductor in photovoltaic modules. Due to its energy-intensive production process and lack of sustainability in the production, it is a relevant issue for circular economy approaches. The processes related to polysilicon (poly-Si) production are responsible for most of the total PV module-related impact on the Global Warming Potential [21].

This study aims to assess circularity measures of polysilicon in the PV supply chain and to measure how the implementation of circular solutions influences the performance indicators. Complementary, Life Cycle Assessment is used for estimating the most relevant environmental impact categories. Therefore, this study aims to present an assessment example that can be used as an aid to decision-makers to guide technology development.

2 Methodology

2.1 Functional unit

The functional unit (FU) used in the study is 1 MWh of electricity produced by a PERC p-type mono-Si photovoltaic module under global average irradiation conditions. This functional unit allows for the consideration of the lifetime among different scenarios. The main parameters related to the functional unit displayed in Table 1.

2.2 Scenario description

Four scenarios based on the combination of technological pathways and circularity options are applied in the research.

– Two technological pathways are examined: 2021 State-of-art PERC and 2032 International Technology Roadmap for Photovoltaic (ITRPV) projection. The data of the IEA PVPS [24] Life Cycle Inventories provide detailed bills of materials for all production steps of the PV module: metallurgical-grade silicon, polysilicon, Czochralski crystal, silicon wafer, photovoltaic cell, and module. The development of production and product utility is assumed on 2032 ITRPV projection. Varying values for parameters (kerf loss, wafer thickness, module efficiency, lifetime) are based on historical data and expected trends from the ITRPV 2022 [25].
– The data for year 2021 from ITRPV [25] is used to model the 2021 State-of-art PERC technological pathway.
– In the case of the 2032 ITRPV projection, it is assumed that improvements are implemented in the wafering process by reducing the kerf loss content and wafer thickness, as well as in the increase of the module efficiency. Values for these parameters are taken from the ITRPV expected trends for the year 2032 [25]. A longer lifetime of the product is assumed (Tab. 2).

Table 2. Four scenarios applied in the study. Based on the combination of 2 technological pathways and 2 circularity options.

	Technology	
Name	2021 State-of-art PERC	2032 ITRPV projection
Kerf loss (μm)	60	43
Wafer thickness (μm)	165	140
Module efficiency (%)	20.9	22.5
Polysilicon consumption (g/Wp)	2.59	1.96
Lifetime (years)	25	35
	Circularity	
Name	Business-as-usual	Closed-loop
EOL collection rate	None	85%
Microsilica from MG-Si production	Used externally	
Internal recycling	Slabs, tails and, tops from ingot cropping recovered and re-used in Cz ingot growth	
Kerf loss recycling	Used externally	Recovered as metallurgical grade silicon and fed into poly-Si production (efficiency – 65%)
End-of-life recycling	No silicon recovery	FRELP technology. Recovered as metallurgical grade silicon and fed into poly-Si production (efficiency – 95%)
	Scenario	
	Technology	Circularity
Scenario 1 (S1)	2021 State-of-art PERC	Business-as-usual
Scenario 2 (S2)	2021 State-of-art PERC	Closed-loop
Scenario 3 (S3)	2032 ITRPV projection	Business-as-usual
Scenario 4 (S4)	2032 ITRPV projection	Closed-loop

– Other parameters and assumptions related to material flows and losses (production yields, collection rates, recycling efficiencies, etc.) are assumed constant among the different scenarios.
– Two circularity options are applied in this study. Potential for internal or external use exists for wastes of production and at the EOL stage. Waste treatment options are designed based on the technological, economic, and legislative conditions working in the field [13,26–30].
– The option "Business-as-usual circularity" represents the current situation in the industry, which is based on economic reasons and legislation requirements. The Waste of Electrical and Electronic Equipment (WEEE) Directive regulates the EOL waste treatment of PV in the European Union [31]. According to the Directive 85% of PV waste must be recovered and 80% prepared for reuse and recycled. However, silicon treatment is not mandatory and thus usually unimplemented in recycling processes. The lack of economic benefits and low mass fractions compared to the front glass or the aluminum frame leads to low recovery rates of PV silicon in practice.
– The "Closed-loop circularity" option represents an example of improved Si recovery, which allows silicon to be used again circularly for new PV polysilicon production. Kerf loss recovery to MG-Si purity silicon is possible with thermal plasma, carbothermic reduction, or inductive melting methods [32–34]. A selected End-of-life technology – FRELP – Full Recovery End of Life Photovoltaic [35], allows for the recovery of silicon from solar cells with a purity of metallurgical-grade silicon.

Table 2 presents the main scenario parameters conducted in the research. Since the collection rates of kerf loss and EOL waste are assumed to be constant, a sensitivity analysis was conducted to assess the contribution of the waste collection rates. The results are given and interpreted in Section 3.3.1.

2.3 Indicators

The assessment is carried out using the following methodologies: Material Circularity Indicator (MCI) for the circular economy approach and Life Cycle Assessment (LCA) to assess the potential environmental impact, that can be allocated to silicon in a PERC p-type mono-Si PV module.

2.3.1 Material Circularity Indicator

The methodology of Material Circularity Indicator was introduced by the Ellen MacArthur Foundation in 2015 and developed in 2019 [15]. The MCI can be applied at material, product, or company levels for quantitative circularity assessment. The indicator is essentially constructed from a combination of three product characteristics [15]:

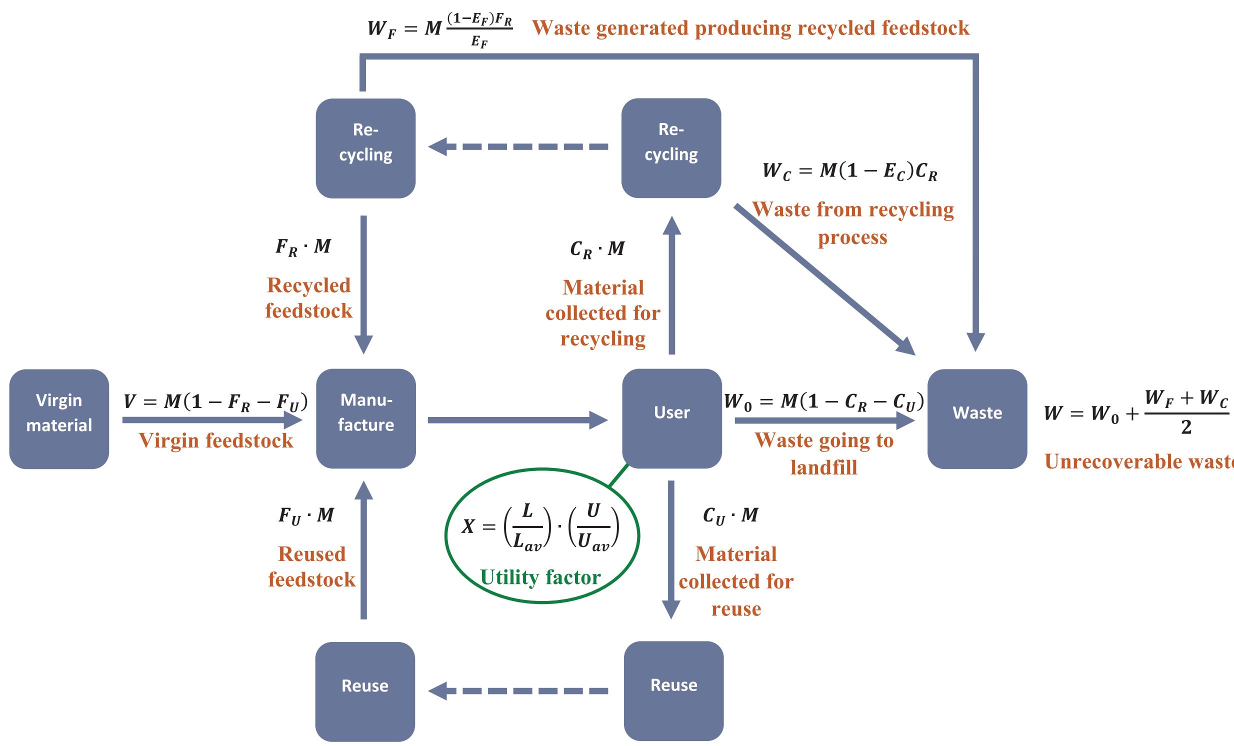

Fig. 1. Schematic representation of material flows MCI.

- Mass V of virgin raw material used in manufacturing.
- Mass W of unrecoverable waste that is attributed to the product (W_0 – uncollected waste, W_C – waste generated in the recycling process; W_F – waste generated to produce any recycled content to use as a feedstock).
- Utility factor X that accounts for the length and intensity of the product's use.

The MCI is applicable to all kinds of physical products, provided the bill of materials is known [15]. This means that the influence of different material compositions on circularity can be easily assessed and compared. The MCI can further be combined with other sustainability indicators and metrics such as criticality ones, thus enabling a more comprehensive approach [36]. The Material Circularity Indicator provides an insight into the amount of circulated material in a product. It can be assessed considering all material flows related to the product. Figure 1 represents the material flows influencing the Material Circularity Indicator.

Based on material flows, the Linear Flow Index (LFI) can be computed. The LFI measures the proportion of material flowing in a linear fashion. The index takes a value between 0 and 1, where 0 is a completely restorative flow and 1 is a completely linear flow [15]. The LFI is calculated as follows:

$$LFI = \frac{V+W}{2M + \frac{W_F - W_C}{2}}. \quad (1)$$

The other key parameter considered in the MCI is the utility X of a product. The utility X is derived from the lifetime and functional units of a product compared to an industry-average product of the same type (Fig. 1).

The Material Circularity Indicator of a material or product can be defined by considering the Linear Flow Index of the product and a factor (X), built as a function F of the utility X that determines the influence of the product's utility on its MCI. The equation used to calculate the MCI of a product is

$$MCI_p^* = 1 - LFI \cdot F(X) \quad (2)$$

where F takes the form:

$$F(X) = \frac{0.9}{X}. \quad (3)$$

MCI takes, by convention, the value 0.1 for a fully linear product (i.e., $LFI = 1$) whose utility equals the industry average (i.e., $X = 1$), while MCI value of 1 presents totally circular material flow [15].

2.3.2 Life Cycle Assessment

In the methodology of Life Cycle Assessment, the environmental impacts of a product or service are investigated over its entire life cycle, providing insight on improvement possibilities as well as crucial information for decision makers [37]. LCAs are standardized the DIN EN ISO 14040 and 14044 [37,38] and follow four major steps in an iterative process: (1) goal and scope definition, (2) inventory analysis, (3) impact assessment, and (4) interpretation. The IEA [39] and the European Commission [40] provided further guidance on LCAs of PV modules and systems specifically.

In analogy to the MCI calculation, the goal of this LCA is to investigate the environmental impacts that can be allocated to the silicon in a p-type mono-Si PV module. The chosen functional unit is 1 MWh of produced electricity, as

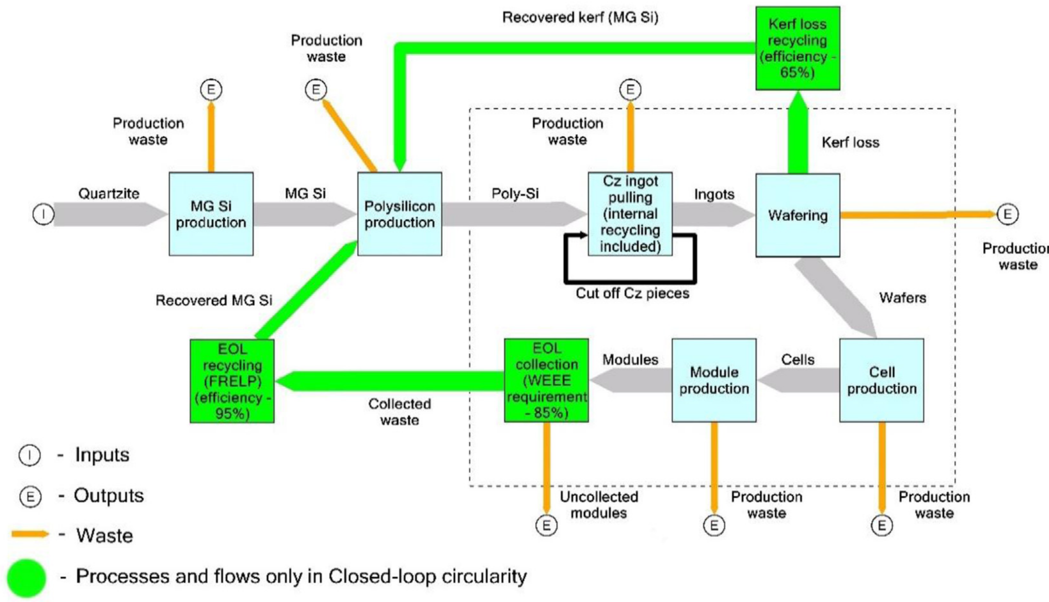

Fig. 2. Supply chain for poly-Si applied in the study.

this allows for the consideration of the lifetime among different scenarios. Various lifetimes and their effects on the LCA results are presented with a sensitivity analysis in Section 3.3.2. While the MCI analysis includes a cradle to grave approach, the LCA is based on a cradle to gate analysis, including the process steps from raw material extraction to the finished PV module. In the LCA, the recycled content is included to account for the improved circularity scenarios, however, the emissions of possible recycling processes are not, due to a lack of data. Further, the LCI is adjusted to fit the MCI scope of analysis more closely, so that only the impacts allocated to the silicon within the PV module are included.

The chosen system model is cut-off. Here, recycled materials are assumed to be burden-free, as their impacts are allocated to their previous life cycle [41]. Any materials in the PV module other than silicon (for example the frame, or metallization pastes) are excluded from this analysis. Auxiliaries such as electricity and heat are included on a weight-ratio-basis, meaning that the weight fraction that the silicon has in a PV module, cell, or wafer was applied to calculate the allocated auxiliary inputs. Any balance-of-system components are out of scope in this study. The location of the production is assumed to be China.

As recommended in the Product Environmental Footprint Category Rules (PEFCR) the chosen impact assessment methodology is EF3.0 [40]. The results are presented in the form of weighted impact scores (endpoint) to allow for the aggregation into a single score. The EF3.0 method covers 16 impact categories. Midpoint results (characterization) are included in the Supplementary Information. Additionally, the impact category *Climate Change* is investigated in more detail, as it is one of the most robust indicators and has the highest contribution to the final single score result.

2.4 Life Cycle Inventory

The study includes all the material flows starting from quartzite to the End-of-life treatment. Yet, the values of virgin material and unrecoverable waste in the results section are expressed by the product of polysilicon. This is a more common index in the PV field. Figure 2 depicts the polysilicon supply chain considered in the study.

As indicated previously, the focus lies on the silicon in the investigated PV module, which is why the consecutive processes (wafer, cell and panel production) have been adjusted to exclude other materials of the module. The data is further adjusted according to the four investigated scenarios. Tables A1–A4 in Appendix A display the material flows for all scenarios.

3 Results

3.1 Material Circularity Indicator

The MCI results for the different scenarios are given in Table 3.

As mentioned above the Linear Flow Index presents how linear the material flows are. The LFI result for Business-as-usual circularity is 0.52 both for 2021 State-of-art PERC and 2032 ITRPV projection. Production efficiency remains the same in most of the processes despite the technological pathway. The only change is assumed for the development in the wafering process – the reduction of waste (kerf loss) accounts for around 3% in the 2032 ITPRV projection. Linear Flow Index for Closed-loop circularity option amounts to 0.22, corresponding to high circularity. Still, there is a potential for improvement in the waste treatment. Recycling efficiency for kerf is still low in Closed-loop circularity. This value of 65% generates a significant amount of unrecoverable

Table 3. Results of MCI (FU = 1 MWh) and its parameters.

SCENARIO	Technology	Circularity	MATERIAL FLOW PARAMETERS			UTILITY PARAMETERS		MCI
			Virgin material (g/MWh)	Unrecoverable waste (g/MWh)	Linear Flow Index	Lifetime (years)	Utility	
Scenario 1 (S1)	2021 State-of-Art PERC	Business-as-usual	86.6	65.1	0.52	25	1	0.54
Scenario 2 (S2)		Closed-loop	38.8	27.1	0.22	25	1	0.80
Scenario 3 (S3)	2032 ITRPV Projection	Business-as-usual	48.0	37.1	0.52	35	1.4	0.67
Scenario 4 (S4)		Closed-loop	21.4	15.1	0.22	35	1.4	0.86

waste. Another point is the collection rate of EOL waste (85%). This requirement is given by the European Union. Grid-connected photovoltaics systems are registered, which should help increase traceability for EOL photovoltaics.

The second component that influences the MCI score is product utility. The 2032 ITRPV projection scenario declares a longer lifetime (35 years) that increases the utility (X) to 1.4. Regardless of the choice of technological scenario, LFI scores remain the same. Therefore, only the higher utility ratio leads to higher MCI results: 0.54 to 0.67 and 0.80 to 0.86 for Business-as-usual and Closed-loop options, respectively. A longer lifetime satisfies one of the three circular economy principles – to keep products or materials in use. Some PV manufacturers already guarantee longer lifetimes for their products than 25 years.

The relatively high MCI result of 0.54 for the scenario 2021 state-of-art PERC/business-as-usual case is mainly due to the reuse of the ingots' sidewall slabs, tails, and tops that are cut-off to form the polysilicon brick from an ingot. These pieces are remelted into the Cz ingot and, due to high collection and internal recycling rates, have a significant impact on the MCI result. Under closed-loop circularity, additionally both the kerf loss and silicon from the EOL waste are recycled. Of note, the business-as-usual option does not cover any end-of-life waste treatment for silicon recovery, while closed-loop presents recycling with a high efficiency of 95% according to FRELP [35]. Furthermore, EOL waste recovered as metallurgical-grade silicon reduces the demand for virgin material. Even if Business-as-usual circularity ensures higher recycling efficiency regarding the kerf loss, recovered material is used externally and it does not contribute to a reduction of virgin material mass. In the closed-loop option kerf loss is recovered as metallurgical-grade silicon and is used for new polysilicon production.

As the MCI is not based on resource efficiency, but on the mass of virgin/waste ratio, additional indicators are required to assess the sustainability of each scenario in more depth. The MCI methodology allows to calculate the mass of virgin material and unrecoverable waste associated with a product. These values flows are also presented in Table 3. Under the technological pathway 2032 ITRPV projection (S3 vs. S1; S4 vs. S2) 43–45% reduction of virgin polysilicon demand and unrecoverable silicon waste is achieved. Closed-loop circularity (S2 vs. S1; S4 vs. S3) reduced the demand for virgin material by 55% and by 59% for unrecoverable waste in comparison to Business-as-usual circularity. The amount of unrecoverable waste is reduced by 5 times in the EOL waste step with Closed-loop circularity (Tables A1–A4 in Appendix A). As the recovered material is used for new polysilicon production, it significantly reduces the mass of virgin material as well.

3.2 Life Cycle Assessment

Figure 3 presents the single score results per scenario (FU = 1 MWh, Method – EF3.0). Furthermore, the contributions of the different impact categories are visualized. It is shown that scenario 1 causes the largest environmental impact in this comparison, followed by scenarios 2, 3, and 4, in that order. The single score for scenario 4 is about 51% lower than for scenario 1. The improved circularity decreases the environmental impacts by around 12%. While the relative contribution of the different impact categories to the single score results is mostly the same across scenarios, some patterns can be identified. At least two-thirds of the single score impacts in all scenarios are due to *Climate Change; Water use; Resource use, fossils*, and *Ecotoxicity, freshwater* categories. The results indicate that technological development has a more significant influence on the result, reducing the impacts by around 46% regardless of the circularity option. The 2032 ITRPV Projection scenarios ensure higher built-in material efficiencies, which are directly related to lower production volumes. This indicates that the technological development ensuring a longer lifetime and higher efficiency has a bigger effect on the single score result than the reduction of virgin material processing.

The cause of the specific impact categories can be further investigated. For instance, Figure 4 shows the *Climate Change* impacts (midpoint) for all scenarios. The carbon footprint of the silicon in the PV module for 1 MWh of produced electricity is 14.25, 13.06, 8.02, and 7.28 kg CO_2 eq. for scenarios 1, 2, 3, and 4, respectively. Half of these impacts originates from the silicon production mix. This includes all impacts from the raw material extraction to the single crystal production in the Cz ingot pulling. The production location is China. Most of the impacts caused in the silicon production mix can be traced back to the electricity consumption in the supply chain, as it is an energy-intensive process and the Chinese electricity mix relies heavily on coal-fired power plants. About 5.79 kg CO_2 eq./MWh is due to the electricity

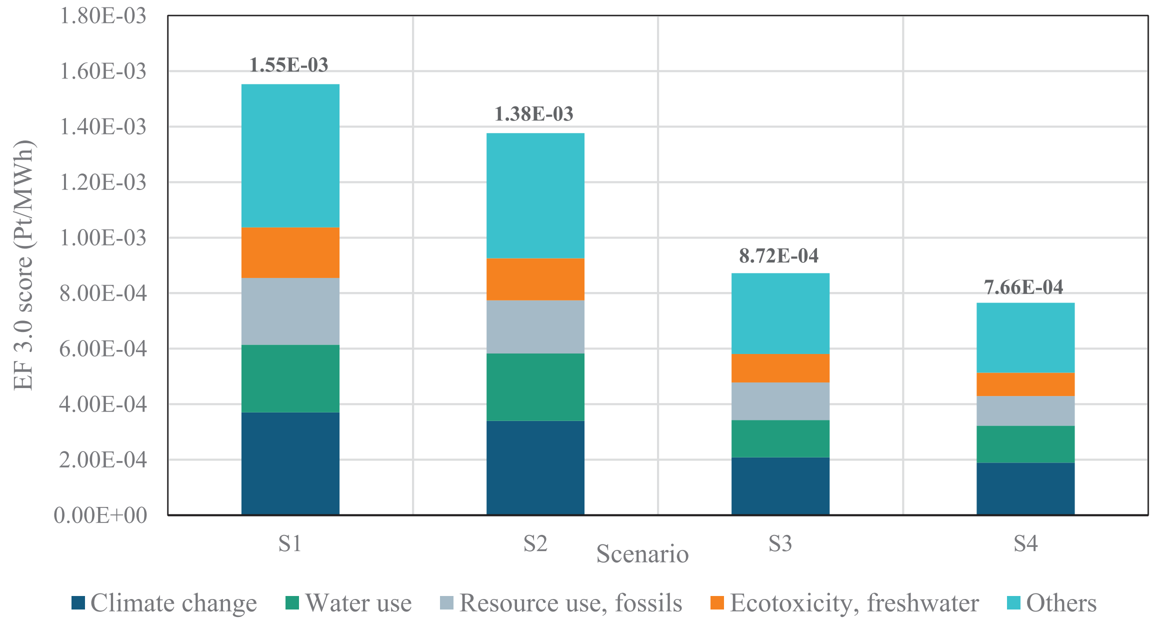

Fig. 3. Normalized and weighted EF3.0 single score results of environmental impacts by categories for silicon used within the PV module in scenarios 1–4.

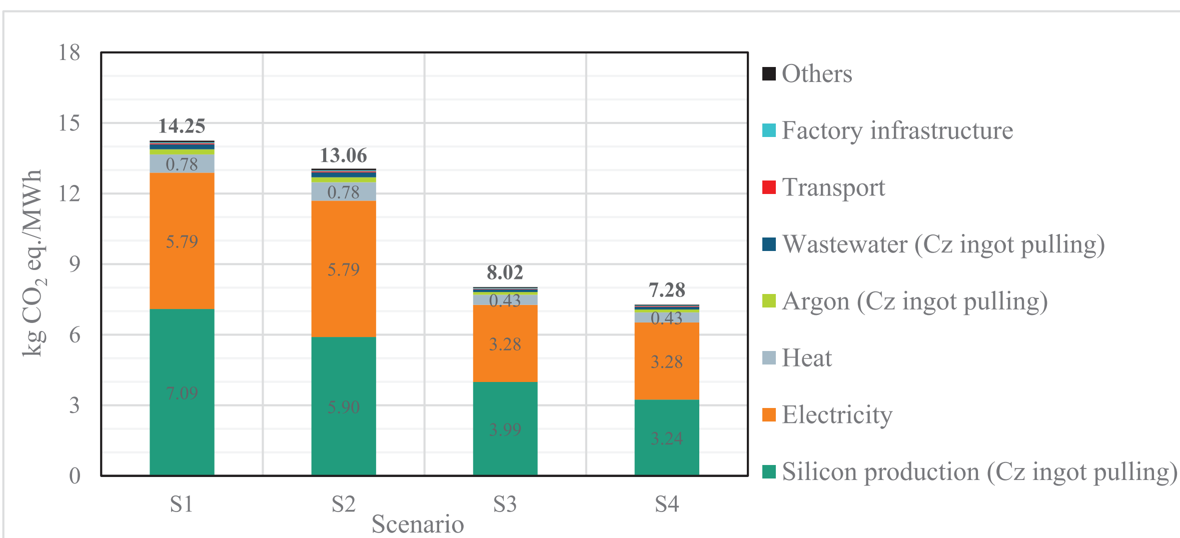

Fig. 4. Climate change impacts for scenarios 1–4 (for silicon within the PV module).

consumption and 0.78 kg CO_2 eq./MWh is caused by the heat consumption in the cell, wafer, and module production processes in scenarios 1 and 2. Both, the electricity and heat consumption impacts are reduced equally for scenarios 3 and 4 to 3.28 kg CO_2 eq./MWh and 0.43 kg CO_2 eq./MWh, respectively.

The LCA results indicate that the 2021 State-of-art PERC/Business-as-usual scenario (S1) has the largest environmental impact in this comparison. Silicon production and the electricity used along the production line are the main sources of impact in all scenarios. The reduction in the energy and silicon consumption across the scenarios has therefore a substantial influence on the respective LCA results. Scenarios 2 and 3 cause fewer environmental impacts per MWh than scenario 1. When comparing scenarios 2 and 3, it becomes clear, that technological improvement with Business-as-usual circularity outperforms the 2021 State-of-art PERC with improved circularity. The increase in electricity production due to the elongated lifetime and higher efficiency has a greater impact on the impacts per MWh than the Closed-loop circularity. In scenario 4, where both improvements are combined, the environmental impacts are reduced by about 50% compared with the original design in scenario 1.

The improvements in the *Climate change* impact category among the scenarios (from 1 to 4) are mostly due to the reduced electricity consumption and the lower demand for silicon. As shown in Figure 3, the *Water use* category also has a high impact on the overall single score results. Also, the impacts in this category are significantly

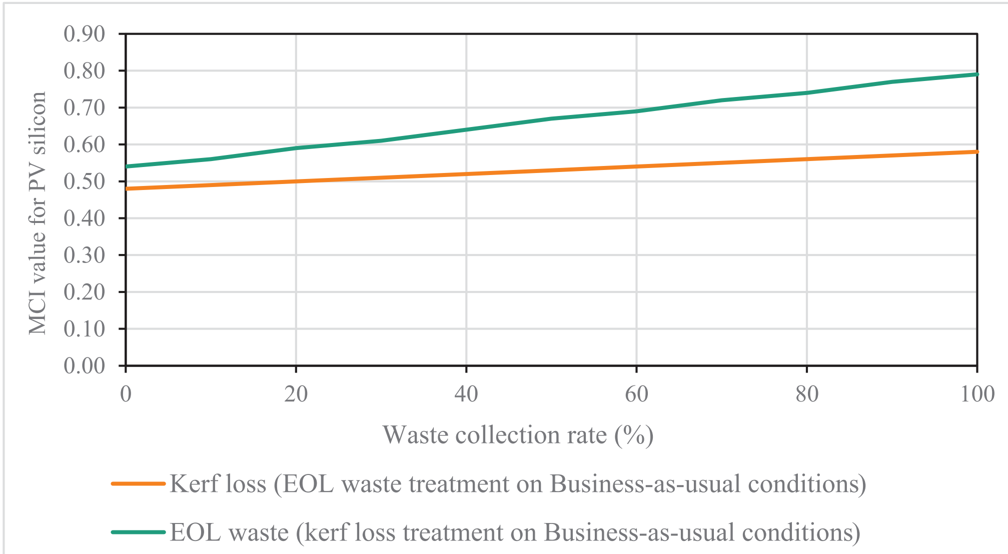

Fig. 5. PV module waste collection rate effect on the MCI score of silicon within the PV module.

influenced by the reduction in silicon demand, across the four investigated scenarios. The Cz ingot pulling in the silicon production is the main cause of water consumption in the production of a PV module. While in scenario 1, the water use amounted to 32.8 m^3 depriv./MWh[1], this is reduced by the scenario 4 to 18 m^3 depriv./MWh[1].

3.3 Sensitivity analysis

3.3.1 Collection rates of kerf loss and End-of-life waste

The Closed-loop circularity option includes an improvement in both, kerf loss and End-of-life waste treatment. These wastes have the biggest impact on the Material Circularity Indicator value due to their high mass. However, separated impacts of waste were not investigated. The sensitivity analysis shows how the MCI evolves with the collection rates of kerf loss and EOL wastes. The MCI was calculated varying kerf loss collection rates under Closed-loop circularity conditions, all other parameters being set constant as per the Business-as-usual circularity option. The same was done for varying EOL waste collection rates. The results of the analysis are presented in Figure 5.

Setting the collection rate of kerf loss to 0% leads to an MCI score of 0.48, which is lower than scenario 1 (0.54). The MCI score for 100% of the collected kerf loss is 0.58. No collection of EOL waste already corresponds to the MCI of scenario 1. An increased End-of-life collection rate presents the highest score of MCI to 0.79 when a collection rate of 100% is assumed. The collection of EOL waste has a higher impact on the Material Circularity Indicator than the kerf loss collection, because of its higher mass and recycling efficiencies.

3.3.2 Lifetime of the PV module

As the extended lifetime and the corresponding higher electricity production in scenarios 3 and 4 have a significant influence on the result, the lifetime effect is tested in a sensitivity analysis. Here, it is assumed that the lifetime electricity production of all modules across the four scenarios is equal. The results are presented in Figure 6. It can be observed that the single score results of the four scenarios are closer together. However, the trend remains clear: the module in scenario 1 causes higher environmental impacts than in 2, 3, and 4 in that order. The improvement from scenario 1 to 4 is at roughly 25% if the electricity output of all systems is assumed to be equal. This means, that half of the environmental footprint reduction that is achieved by changing from the S1 setup to S4, can be attributed to the extended lifetime, while the other half is due to the optimized processes and increased module efficiency.

4 Discussion

The methodology of the Material Circularity Indicator applied in the research provides a detailed assessment of material flows circulations. Still, it must be discussed in some critical arguments in terms of circular economy principles. One of the main CE goals is to lessen inputs. However, the MCI as a metric is based on a mass proportion of waste and recovered material. This means that high collection and recovery rates of wastes within production steps increase the overall MCI value of the product. This can be illustrated with an example from the study. Poly-Si ingots are cut-off to form the shape of the wafers. A significant amount of polysilicon is created as slabs, tails, and tops. However, all these parts are remelted again to the Cz crystal. Following the methodology, these steps significantly increase the MCI score of polysilicon. Nevertheless, this contradicts the idea of circular economy to use fewer resources [44]. More efficient technological alternatives could replace the traditional production e.g., fluidized bed reactor instead of Siemens process in poly-Si production or epitaxial wafering instead of diamond wire sawing. The chance to increase circularity by creating not irrelevant waste

[1] In the EF3.0 methodology, the water use is quantified as "user deprivation potential" (m^3 depriv./functional unit) [42,43].

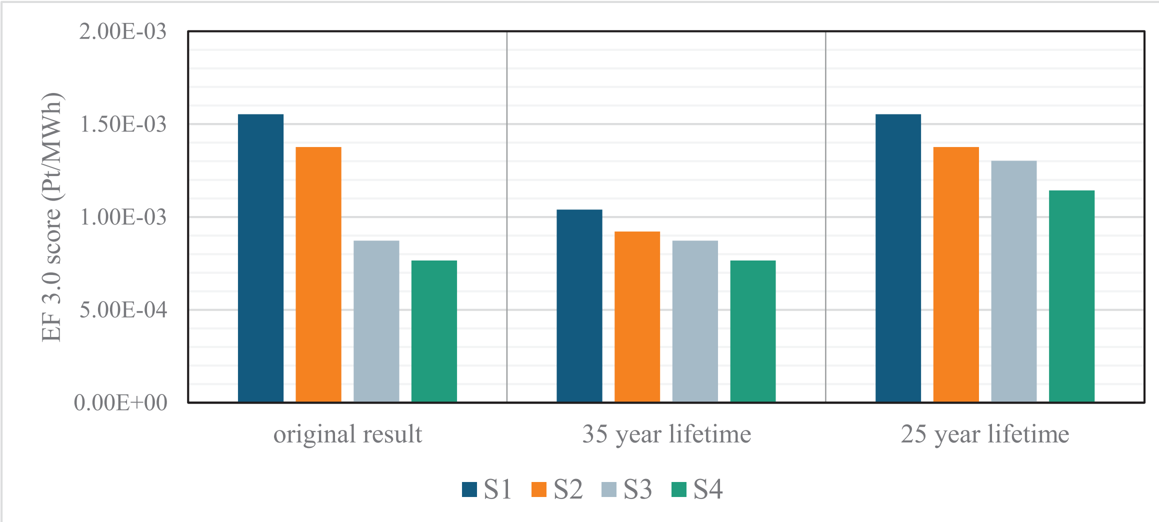

Fig. 6. Lifetime effect to normalized and weighted EF3.0 single score LCA results (for silicon within the PV module only).

and reusing it could be an example of so-called "circular washing". This strategy is used by companies to present goods as produced in a circular economy style.

Another critical point of the MCI methodology is related to the internal or external use of the recycled material. Circular economy is a systems-thinking strategy expanding product-level boundaries. Internal recycling reduces demand for virgin material, however, in some industries it's not simple to achieve this. Polysilicon production for PV requires high purity and a specific consistency of the material. These requirements are not easy to satisfy with recycled wastes from production or EOL. Cleaning with hazardous materials and various methods are needed to recover silicon to be ready for PV production again. These needs create an additional impact on the environment and reduces the recycling yield. Yet, there is a high demand for lower quality silicon alloys in other industries. Nevertheless, the MCI methodology benefits internal circularity due to decrease in mass of virgin material.

Universal metrics joining circularity and environmental impacts would be useful to compare the scenarios' sustainability performances. Few methodologies were tested to obtain a single, composite score in the research. Mantalovas and Di Mino proposed the Environmental Sustainability and Circularity Indicator (ESC_i) [20]. It combines the MCI scores with the normalized and weighted results of LCA to transform those into one unitless number. The formula describing the indicator can be seen in equation (4) [20]:

$$\mathrm{ESC_i} = \frac{1}{LCA_T^{(1-MCI)}} \times 100. \tag{4}$$

The higher the result, the more preferable the scenario is in terms of circularity and environment. However, the contribution of each parameter remains unclear to the combined score. Besides, the ESC_i result is easily manipulated – when the LCA result is below 1, a higher MCI score reduces the ESC_i result, and therefore a false interpretation.

It must be pointed out that there are also some limitations to this LCA conducted. As described in the methodology, the MCI analysis includes a cradle to grave approach, whereas the LCA is based on a cradle to gate analysis. While the LCA accounts for the recycled content, the emissions of possible recycling processes are not considered, due to a lack of available data. Additionally, adjustments were made to the LCI to fit the scope of the MCI-analysis more closely. Therefore, only the impacts allocated to the silicon within the PV module are included, whilst any other materials (for example the frame, or metallization pastes) that are part of a PV module have not been investigated. Auxiliaries, such as electricity, heat and transport have been included on the basis of a weight-ratio. This entails uncertainty and can influence the result. Finally, the normalization and weighting of the characterized results introduce additional uncertainty. However, to achieve a single score for the respective scenarios and make them more easily comparable, this step was taken. In order to give full transparency of the results, the respective characterized values are included in Appendix B.

5 Conclusion

Photovoltaic solar modules have a major impact on achieving long-term climate change goals. Forecasted projections for terawatt-scale deployment require large amounts of materials. Concerns about resource efficiency, waste treatment, virgin material need, or environmental impacts are pressing topics in the field. Some materials, i.e., silicon, play an important role, due to its irreplaceability, high environmental impact, and challenging sustainability in the supply chain.

In this research, four scenarios based on technological and circular economy principles were created to test the applicability and utility of a circularity metric, combined with an LCA. The methods of Material Circularity Indicator and Life Cycle Assessment were applied to measure the example of polysilicon production for photovoltaics. The results showed that the 2021 State-of-art case of the PV polysilicon supply chain corresponds to the MCI score of 0.54. The higher-than-expected result was achieved mainly by internal recycling. Improved circularity with kerf loss and EOL waste recovery on the closed-loop model significantly increases the overall MCI value up to 0.80. It has been shown that End-of-life waste treatment contributes more to the MCI than the kerf loss treatment, because of the higher mass of waste available from old modules than kerf loss. The effect of circularity on the mass of virgin material and unrecoverable waste has been calculated. The implementation of Closed-loop circularity reduces the need for virgin material by up to 55% and by 59% for unrecoverable waste compared to Business-as-usual circularity. The effect of improved utility on the aforementioned parameters was not so significant. However, the evaluation by life cycle assessment methodology showed that improved utility causes lower environmental impact since it significantly reduces the volume of wafer, cell, and module production. The higher material efficiency was achieved due to optimized production processes, extended lifetime and increased module efficiency.

This study contributes to the research evaluating circular economy approaches in the PV industry. The results highlighted the benefit of joining metrics for circularity and environmental assessment. The interaction between them can be interpreted in the context of sustainability as guidance for the development in photovoltaics.

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Author contribution statement

A.R. Zubas: Conceptualization, Investigation, Methodology, Writing – Original Draft, Review & Editing; M. Fischer: Investigation, Writing – Original Draft, Review & Editing; E. Gervais: Conceptualization, Methodology, Supervision, Review & Editing; S. Herceg: Supervision, Review & Editing; S. Nold: Conceptualization, Methodology, Supervision, Review & Editing.

Appendix A: Life cycle inventories

Tables A1–A4 present the material flows for scenarios.

Nomenclature

$\boldsymbol{E_F}$ Efficiency of recycled feedstock
$\boldsymbol{P'_R}$ Collection rate
$\boldsymbol{F_R}$ Fraction from recycled feedstock
$\boldsymbol{E'_C}$ Efficiency of recycling waste
$\boldsymbol{C_R}$ Collection rate
$\boldsymbol{E_C}$ Efficiency of recycling waste

Table A1. Material flows for 2021 State-of-art PERC/Business-as-usual scenario.

Scenario 1 Built-in Si – 46.6 g/MWh	Input (g)				Feedstock		Waste/loss treatment		Output (g)				Use of recovered material (internal/external)
Production process	Virgin	Recycled	Total input	Yield	E_F	F_R	P'_R	E'_C	Product	Unrecoverable waste	Recovered material	Total output	
MG silicon production*	123.6	0	123.6	0.79	0	0	0.98	0.99	97.9	0.6	24.9	123.6	External
Polysilicon production	97.9	0	97.9	0.88	0	0	0	0	86.6	11.4	0	97.9	
Cz ingot pulling	86.6	62.5	149.2	0.98	0.96	0.42	0	0	146.2	3.0	0	149.2	
Cropping and squaring	146.2	0	146.2	0.55	0	0	0.98	0.96	79.7	2.7	62.5	146.2	Internal
Wafering	79.7	0	79.7	0.68	0	0	0.99	0.7	54.1	4.2	17.7	79.7	External
PERC cells production	54.1	0	54.1	0.88	0	0	0	0	47.6	6.6	0	54.1	
Module assembly	47.6	0	47.6	0.98	0	0	0	0	46.6	1.0	0	47.6	
End-of-life							$\boldsymbol{C_R}$	$\boldsymbol{E_C}$					
Photovoltaic waste	46.6						0	0		46.6	0	46.6	

*The mass of material entering MG silicon production is transformed to mass of silicon in quartzite (SiO_2). Silicon corresponds to around 46.75% weight in quartzite [45].

Table A2. Material flows for 2021 State-of-art PERC/Closed-loop scenario.

Scenario 2 Built-in Si – 46.6 g/MWh	Input (g)				Feedstock		Waste/loss treatment		Output (g)				Use of recovered material (internal/external)
Production process	Virgin	Recycled	Total input	Yield	E_F	F_R	P'_R	E'_C	Product	Unrecoverable waste	Recovered material	Total output	
MG silicon production*	55.3	0	55.3	0.79	0	0	0.98	0.99	43.8	0.3	11.1	55.3	External
Polysilicon production	43.8	54.1	97.9	0.88	0.84	0.55	0	0	86.6	11.3	0	97.9	
Cz ingot pulling	86.6	62.5	149.2	0.98	0.96	0.42	0	0	146.2	3.0	0	149.2	
Cropping and squaring	146.2	0	146.2	0.55	0	0	0.98	0.96	79.7	2.7	62.5	146.2	Internal
Wafering	79.7	0	79.7	0.68	0	0	0.99	0.65	54.1	4.8	16.5	79.7	Internal
PERC cells production	54.1	0	54.1	0.88	0	0	0	0	47.6	6.6	0	54.1	
Module assembly	47.6	0	47.6	0.98	0	0	0	0	46.6	1.0	0	47.6	
End-of-life							$\boldsymbol{C_R}$	$\boldsymbol{E_C}$					
Photovoltaic waste	46.6						0.85	0.95		8.0	37.6	47.6	Internal

*The mass of material entering MG silicon production is transformed to mass of silicon in quartzite (SiO_2). Silicon corresponds to around 46.75% weight in quartzite [45].

Table A3. Material flows for 2032 ITRPV projection/Business-as-usual scenario.

Scenario 3 Built-in Si – 26.9 g/MWh	Input (g)				Feedstock		Waste/loss treatment		Output (g)				Use of recovered material (internal/external)
Production process	Virgin	Recycled	Total input	Yield	E_F	F_R	P'_R	E'_C	Product	Unrecoverable waste	Recovered material	Total output	
MG silicon production*	68.5	0	68.5	0.79	0	0	0.98	0.99	54.2	0.4	13.8	68.5	External
Polysilicon production	54.2	0	54.2	0.88	0	0	0	0	48.0	6.2	0	54.2	
Cz ingot pulling	48.0	34.6	82.6	0.98	0.96	0.42	0	0	81.0	1.7	0	82.6	
Cropping and squaring	81.0	0	81.0	0.55	0	0	0.98	0.96	44.2	1.5	34.6	81.0	Internal
Wafering	44.2	0	44.2	0.71	0	0	0.99	0.7	31.2	2.1	9	44.2	External
PERC cells production	31.2	0	31.2	0.88	0	0	0	0	27.4	3.8	0	31.2	
Module assembly	27.4	0	27.4	0.98	0	0	0	0	26.9	0.6	0	27.4	
End-of-life							$\boldsymbol{C_R}$	$\boldsymbol{E_C}$					
Photovoltaic waste	26.9						0	0		26.9	0	26.9	

*The mass of material entering MG silicon production is transformed to mass of silicon in quartzite (SiO_2). Silicon corresponds to around 46.75% weight in quartzite [45].

Table A4. Material flows for 2032 ITRPV projection/Closed-loop scenario.

Scenario 4 Built-in Si – 26.9 g/MWh	Input (g)			Feedstock			Waste/loss treatment		Output (g)				Use of recovered material (internal/external)
Production process	Virgin	Recycled	Total input	Yield	E_F	F_R	P'_R	E'_C	Product	Unrecoverable waste	Recovered material	Total output	
MG silicon production*	30.5	0	30.5	0.79	0	0	0.98	0.99	24.2	0.2	6.2	30.5	External
Polysilicon production	24.2	30.0	54.2	0.88	0.84	0.55	0	0	48.0	6.2	0	54.2	
Cz ingot pulling	48.0	34.6	82.6	0.98	0.96	0.42	0	0	81.0	1.7	0	82.6	
Cropping and squaring	81.0	0	81.0	0.55	0	0	0.98	0.96	44.2	1.5	34.6	81.0	Internal
Wafering	44.2	0	44.2	0.71	0	0	0.99	0.65	31.2	2.4	8.3	44.2	Internal
PERC cells production	31.2	0	31.2	0.88	0	0	0	0	27.4	3.8	0	31.2	
Module assembly	27.4	0	27.4	0.98	0	0	0	0	26.9	0.5	0	27.4	
End-of-life							$\boldsymbol{C_R}$	$\boldsymbol{E_C}$					
Photovoltaic waste	26.9						0.85	0.95		4.6	21.7	26.9	Internal

*The mass of material entering MG silicon production is transformed to mass of silicon in quartzite (SiO_2). Silicon corresponds to around 46.75% weight in quartzite [45].

Appendix B: LCA Characterization results

Table B1. Characterization results per scenario. LCIA method: EF 3.0. Functional Unit = 1 MWh.

Impact Category	Unit	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Climate change	kg CO_2 eq	1.42E+01	1.31E+01	8.02E+00	7.28E+00
Ozone depletion	kg CFC11 eq	3.90E-07	3.44E-07	2.19E-07	1.90E-07
Ionising radiation	kBq U-235 eq	4.48E-01	4.08E-01	2.51E-01	2.26E-01
Photochemical ozone formation	kg NMVOC eq	5.01E-02	4.48E-02	2.82E-02	2.49E-02
Particulate matter	disease inc.	9.50E-07	8.89E-07	5.35E-07	4.96E-07
Human toxicity, non-cancer	CTUh	1.67E-07	1.48E-07	9.41E-08	8.26E-08
Human toxicity, cancer	CTUh	4.25E-09	3.81E-09	2.41E-09	2.14E-09
Acidification	mol H+ eq	7.65E-02	6.90E-02	4.31E-02	3.84E-02
Eutrophication, freshwater	kg P eq	5.39E-03	3.72E-03	3.03E-03	2.06E-03
Eutrophication, marine	kg N eq	2.13E-02	1.92E-02	1.19E-02	1.07E-02
Eutrophication, terrestrial	mol N eq	1.95E-01	1.74E-01	1.10E-01	9.70E-02
Ecotoxicity, freshwater	CTUe	4.05E+02	3.37E+02	2.28E+02	1.88E+02
Land use	Pt	3.98E+01	3.26E+01	2.26E+01	1.83E+01
Water use	m^3 depriv.	3.28E+01	3.27E+01	1.81E+01	1.80E+01
Resource use, fossils	MJ	1.88E+02	1.50E+02	1.06E+02	8.30E+01
Resource use, minerals and metals	kg Sb eq	2.80E-05	2.68E-05	1.65E-05	1.57E-05

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