

## Life cycle assessment of different chalcogenide thin-film solar cells

Shahaboddin Resalati<sup>a,\*</sup>, Tobechi Okoroafor<sup>a</sup>, Amani Maalouf<sup>a</sup>, Edgardo Saucedo<sup>b</sup>, Marcel Placidi<sup>b,c</sup>

<sup>a</sup> Oxford Brookes University, Headington Campus, Gypsy Lane, Oxford, UK, OX30BP

<sup>b</sup> Polytechnic University of Catalonia, Campus Besòs - Building C - 4th Floor, Office C4.2.A, Av. d'Eduard Maristany, 16, 08930 Barcelona

<sup>c</sup> Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, 2a pl., 08930 Sant Adrià del Besòs Barcelona, Spain

### HIGHLIGHTS

- LCA of flexible chalcogenide solar cells were assessed for the first time on cradle-to-gate basis.
- At comparable efficiencies, CIGS and CZGeSe had the highest environmental impacts with Sb<sub>2</sub>S<sub>3</sub> having the lowest.
- Electricity consumption was identified as the environmental hotspot during manufacturing of the cells.
- The absorber layer of the cells contributed the most to the majority of impact categories.
- Considerable environmental benefits were associated with non-toxic chalcogenide cells if efficiency can be improved.

### ARTICLE INFO

#### Keywords:

Thin-film photovoltaic  
Chalcogenide solar cells  
Environmental impact assessment  
Cradle-to-gate  
Life cycle assessment

### ABSTRACT

Thin-film photovoltaics (PV) cells offer several benefits over conventional first-generation PV technologies, including lighter weight, flexibility, and lower power generation cost. Among the competing thin-film technologies, chalcogenide solar cells offer promising performance on efficiency and technological maturity level. However, in order to appraise the performance of the technology thoroughly, issues such as raw materials scarcity, toxicity, and environmental impacts need to be investigated in detail. This paper therefore, for the first time, presents a cradle to gate life cycle assessment for four different emerging chalcogenide PV cells, and compares their results with copper zinc tin sulfide (CZTS) and the commercially available CIGS to examine their effectiveness in reducing the environmental impacts associated with PV technologies. To allow for a full range of indicators, life cycle assessment methods CML 2001, IMPACT 2002+, and ILCD 2011 were used to analyse the results. The results identify environmental hotspots associated with different materials and components and demonstrate that using current efficiencies, the environmental impact of copper indium gallium selenide (CIGS) for generating 1kWh electricity was lower than that of the other studied cells. However, at comparable efficiencies the antimony-based cells offered the lowest environmental impacts in all impact categories. The effect of materials used was also found to be lower than the impact of electricity consumed throughout the manufacturing process, with the absorber layer contributing the most to the majority of the impact categories examined. In terms of chemicals consumed, cadmium acetate contributed significantly to the majority of the environmental impacts. Stainless steel in the substrate/insulating layer and molybdenum in the back contact both contributed considerably to the toxicity and ozone depletion impact categories. This paper demonstrates considerable environmental benefits associated with non-toxic chalcogenide PV cells suggesting that the current environmental concerns can be addressed effectively using alternative materials and manufacturing techniques if current efficiencies are improved.

### 1. Introduction

The reduction of harmful energy-related environmental emissions is

crucial to the energy transformation. Rapidly transitioning the world away from the use of fossil fuels to cleaner renewable forms of energy is essential if the world is to meet the climate targets. In this context, it is proposed that by 2050, energy-related emissions should be reduced by

\* Corresponding author.

E-mail address: [sresalati@brookes.ac.uk](mailto:sresalati@brookes.ac.uk) (S. Resalati).

<https://doi.org/10.1016/j.apenergy.2022.118888>

Received 6 September 2021; Received in revised form 11 February 2022; Accepted 3 March 2022

Available online 11 March 2022

0306-2619/© 2022 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

Nomenclature			
<i>Solar cells</i>			
CdTe	Cadmium telluride	CNG	Carcinogens
CIGS	Copper indium gallium selenide	EP	Eutrophication potential
CIGSSe	Copper indium gallium sulfoselenide	EPBT	Energy payback time
CIS	Copper indium selenide	EPF	Energy production factor
CZGeSe	Copper zinc germanium selenide	Ex	Ecotoxicity
CZTS	Copper zinc tin sulfide	FEP	Freshwater eutrophication
CZTSe	Copper zinc tin selenide	FD	Fossil depletion
PVs	Solar photovoltaics	FWE	Freshwater aquatic ecotoxicity
Sb <sub>2</sub> S <sub>3</sub>	Antimony trisulfide	GW	Global warming
Sb <sub>2</sub> Se <sub>3</sub>	Antimony triselenide	GWP	Global Warming Potential
<i>Chemical compounds</i>		HT	Human toxicity
Ga	Gallium	HTc	Human toxicity, cancer effects
In	Indium	HTnc	Human toxicity, non-cancer effects
Te	Tellurium	IR	Ionizing radiation
Se	Selenium	LCCE	Life cycle conversion efficiency
S	Sulphur	LO	Land occupation
SnS	tin sulphide	LU	Land use
Sb <sub>2</sub> (S,Se) <sub>3</sub>	Antimony selenosulfide	NCG	Non-carcinogens
PbS	lead sulphide	MAE	Marine aquatic ecotoxicity
<i>Nomenclature</i>		MD	Metal depletion
1D	1-dimensional	ME	Mineral extraction
CRM	Critical raw materials	MEP	Marine eutrophication
EU-28	European Union	MFRD	Mineral, fossil and resource depletion
FU	Functional unit	NC	Non carcinogens
LCA	Life cycle assessment	NRE	Non-renewable energy
<i>Impact categories</i>		OD	Ozone depletion
AA	Aquatic acidification	ODP	Ozone layer depletion
ADP	Abiotic depletion	PE	Primary energy
ADPF	Abiotic depletion (fossil fuels)	PED	Primary energy demand
AE	Aquatic eco-toxicity	PENRT	Primary energy non-renewable resource
AEP	Aquatic eutrophication	PERT	Primary energy renewable resource
AP	Acidification potential	PM	Particulate matter
CA	Carcinogens	POF	Photochemical ozone formation
CC	Climate change	POP	Photochemical oxidation
CED	Cumulative energy demand	RE	Respiratory inorganics
		TA	Terrestrial acid/nitrification
		TE	Terrestrial ecotoxicity
		TEP	Terrestrial eutrophication
		WRD	Water resource depletion

70% relative to current levels [1]. As a result, it is anticipated that an increased use of a combination of solar photovoltaics (PV) and other renewable energy technologies would be required to meet this target [2]. Among all low-carbon technology options, rapid deployment of solar PV alone can result in a considerable emission reduction of 4.9 gigatonnes of carbon dioxide (Gt CO<sub>2</sub>) by 2050. This would account for 21% of total emission mitigation potential in the energy sector. To achieve this target, it is expected that by 2050, solar PV would be the second-largest source of electricity and would pave the way for global energy sector change. Solar PV would generate a quarter (25%) of the world's energy demand, becoming the dominant generation source by 2050. This entails a massive increase (almost six-fold) in the total capacity of solar PV over the next 10 years, from a global total of 480 GW in 2018 to 2840 GW by 2030 and a significant 8519 GW by 2050, representing an increase of over eighteen times from 2018 levels [1]. This is evident as the growth of PV technology has regularly outpaced the International Energy Agency's reference scenario estimates and cumulative solar capacity projections made for 2030 have already been met [3]. The deployment of solar PV will continue to break records, with yearly additions reaching 162 GW by 2022, which is about 50% more than pre-pandemic level of 2019 [4,5]. The European Commission has also announced a change of the Renewables Directive in 2018, which sets a

binding objective of 32% renewable energy sources by 2030 [6,7]. As a result of these trends, PV technologies have the potential to supply a considerable portion of the future energy mix, making them particularly appealing as they contribute to the world's environmental sustainability and energy security issues, thus, playing a major role in national and international energy strategies [3].

PV cells are generally categorised into three generations of technologies. The first generation refers to the conventional crystalline silicon base structure, as single and multi-crystalline silicon cells. The second generation refers to the thin-film solar cells, which include amorphous silicon and chalcogenide cells such as cadmium telluride (CdTe), copper indium gallium selenide (CIGS)/copper indium selenide (CIS) and copper zinc tin sulfide (CZTS). Chalcogenide solar cells have absorber layers made up of chalcogenides, which are compounds consisting of chalcogen elements such as sulphur (S), selenium (Se) and/or tellurium (Te) [8]. The third generation technologies include concentrator PVs, organics, dye-sensitized solar cells, tandem devices and others [9].

Crystalline silicon cells have the majority of market share due to their high efficiency [10] and technological advancement. Among the different emerging inorganic solar cells aiming to claim market share from crystalline silicon cells in the future [11], chalcogenides currently

represent the most promising ones, especially from an efficiency and technological maturity point of view. This family of materials range from single elemental Se to binaries (CdTe, tin sulphide (SnS), Antimony selenosulfide (Sb<sub>2</sub>(S,Se)<sub>3</sub>), lead sulphide (PbS)) and multinary compounds (Copper indium gallium sulfoselenide (CIGSSe), CIGS and copper zinc tin sulfoselenide (CZTSSe)). CIGS and CdTe are already commercially available, having clearly demonstrated high performance (greater than 22% at cell level) and are successfully deployed on an industrial scale [11]. This already established technology is clearly an advantage for emerging chalcogenide absorbers, which can benefit from pre-existing manufacturing infrastructure. In that sense, kesterites and antimony chalcogenides demonstrated promising efficiencies (12.6% for CZTSSe and 9.9% for Sb<sub>2</sub>(S,Se)<sub>3</sub>). They are formed from earth-abundant and non-toxic (or less toxic) constituents with similarities to CIGS and CdTe including the manufacturing steps shown in Table 1 [11]. Both materials have shown excellent properties as photovoltaic absorbers, very high light absorption coefficient (above 10<sup>5</sup> cm<sup>-1</sup>), natural p-type conductivity, and their bandgap can be tuned with the composition. Moreover, the quasi 1-dimensional (1D) structure of the antimony chalcogenides confers them the particularity of controlled anisotropic optical, electrical and structural properties [12].

Table 2 presents a summary of published LCA focusing primarily on chalcogenide thin film PV cells. The research articles included mostly well-known chalcogenides such as CdTe, CIGS, CIS and CZTS. CIGS/ CIS have the majority of the market share of the thin film PV market with CdTe accounting for only 5% and CZTS yet to attain mass production [13]. This is also evident in the LCA studies as the majority of studies have been conducted focusing on CdTe, CIGS and CIS. The majority of these studies are conducted in Europe with most studies limiting the scope of their environmental indicators to GWP and CED. This could have the potential risk of not assessing the possible shift of environmental burdens from GWP to other environmental impact categories. A careful analysis of these studies indicate that majority of the impact is due to electricity use during production of the thin film PV cells. It has also been highlighted that additional energy consumption is required after decommissioning of CIGS, CIS and CdTe for the processing and recycling of the toxic material contained in their absorbers further highlighting the need for alternatives such as CZTS and the other non-toxic chalcogenide cells.

**Table 1**  
Probable industrial manufacturing process for CZTS, CIGS and CdTe photovoltaic cell (adapted from Collier et al. [18]).

Manufacturing Steps	Copper zinc tin sulphide (CZTS)	Copper indium gallium selenide (CIGS)	Cadmium telluride (CdTe)
1	<b>Substrate:</b> Cleaning	<b>Substrate:</b> Cleaning	<b>Substrate:</b> Cleaning
2	<b>Back contact:</b> Sputtering of Mo	<b>Back contact:</b> Sputtering of Mo	<b>Front contact:</b> Vapour transport deposition of tin oxide
3	<b>Absorber layer:</b> Co-sputtering of Cu, Zn, Sn	<b>Absorber layer:</b> Co-evaporation of Cu, In, Ga	<b>Window layer:</b> Vapour transport deposition of CdS
4	<b>Absorber Layer:</b> Selenisation or Sulfurization	<b>Absorber Layer:</b> Selenisation	<b>Absorber Layer:</b> Vapour transport deposition of CdTe
5	<b>Buffer Layer:</b> Chemical bath deposition of CdS	<b>Buffer Layer:</b> Chemical bath deposition of CdS	<b>Back contact:</b> Sputtering of IZO
6	<b>Intrinsic layer:</b> Sputtering of IZO	<b>Intrinsic layer:</b> Sputtering of IZO	<b>Back Contact:</b> Sputtering of AZO
7	<b>Window Layer:</b> Sputtering of AZO	<b>Window Layer:</b> Sputtering of AZO	<b>Back Contact:</b> Thermal Evaporation of Al
8	<b>Front contact:</b> Thermal Evaporation of Al	<b>Front contact:</b> Thermal Evaporation of Al	

**Table 2**  
Summary of existing chalcogenide thin-film solar cells LCA studies.

Technology	Reference	Life cycle stages	Impact categories	Location	PCE (%)
CdTe	[40]	Cradle to gate	GWP, CED	South-European	9
CdTe	[2]	Cradle to gate	AP, ET, EP, GWP, HT, HTC, HTnC, ME, FEC, WD	USA	NA
CdTe	[41]	N/A	GWP, CED	South-European	10.9
CdTe	[42]	Cradle to gate	GWP, CED	USA	9
CdTe	[43]	N/A	GWP	South-European	10.9
CdTe	[44]	End-of-Life	CED	Italy	-
CdTe	[45]	Cradle to grave	GWP, CED, AP, EP, POC	Europe	10.9
CdTe	[45]	Cradle to grave	GWP, CED, AP, EP, POF	Europe	10.9
CdTe	[46]	Cradle to grave	GWP, CED	China	11
CdTe	[47]	Cradle to grave	GWP, CED	China	22
CdTe	[48]	Cradle to grave	EPBT, GWP, AP, EP, ODP	UK	5–10
CdTe	[49]	Cradle to gate	GWP, CED	Japan	10
CdTe	[50]	Cradle to gate	GWP, FD, EPBT, CO <sub>2</sub> PBT	Korea	11.2
CdTe	[51]	N/A	EPBT, EPF, LCCE	India	
CdTe	[52]	Cradle to gate	GWP, AP, FEC	South-European	9
CdTe	[52]	Cradle to gate	GWP, AP, FEC	South-European	9
CdTe, CIGS	[53]	N/A	GWP, MD, LO, CNG, FWE, NCG, EP, Ex, POP, FD, AP	USA	11.6–20.8
CdTe, CIGS	[9]	Cradle to gate	CED, GWP, AP, ODP	Switzerland	14–17
CIGS	[9]	N/A	GWP, CED	South European	10.5
CIGS	[10]	Cradle to gate	GWP, CED	China	12
CIGS	[10]	Cradle to gate	GWP, CED	N/A	12
CIGS	[54]	Cradle to gate	ReCiPe indicators	Finland	15
CIGS	[55]	Cradle to gate	GWP	Netherlands	15
CIS	[46]	Cradle to grave	GWP, CED	China	11
CIS	[47]	Cradle to grave	GWP, CED	China	11
CIS	[56]	Cradle to grave	GWP	Switzerland	10.7
CIS	[52]	Cradle to gate	GWP, AP, FEC	South-European	11
CIS	[52]	Cradle to gate	GWP, AP, FEC	South-European	11
CZTS	[18]	Cradle to gate			10

(continued on next page)

Table 2 (continued)

Technology	Reference	Life cycle stages	Impact categories	Location	PCE (%)
CZTS	[57]	Cradle to gate	GWP, CED, FU, ET	United States	15
		Cradle to gate	CC, HT, ET	Europe	

No existing published work investigate the environmental impact of emerging chalcogenide solar cells such as Copper zinc tin selenide (CZTSe), Copper zinc germanium selenide (CZGeSe), Antimony triselenide ( $Sb_2Se_3$ ) and Antimony trisulfide ( $Sb_2S_3$ ). In this paper we aim to address this shortcoming by conducting, for the first time, a comprehensive LCA on these chalcogenide cells alongside CZTS and the commercially available CIGS (the results of CIGS and CZTS LCA models are compared with existing studies in the following sections). A selective, but not exhaustive list of LCA research studies on chalcogenide thin film PV technology is presented in Table 2 highlighting the need for a thorough LCA on other emerging chalcogenide cells. Most of the aforementioned studies conducted LCA on a cradle-to gate or a cradle-to-grave system boundary with limited environmental impact categories assessed. To that purpose, the LCA in this study is carried out in an integrated framework, from cradle to gate, and across numerous environmental impact categories, including human toxicity impact, not emphasized in most of the LCA studies. Characterising the effect to human health is important as the production of some materials such as stainless steel used in cell fabrication may cause some concern due to the use of highly toxic chemicals [14]. Such analyses can assist solar cell manufacturers and researchers in reducing the associated environmental impact of emerging technologies through identifying the hot-spots in relation to key impact categories such as ozone and abiotic depletion, global warming potentials, marine aquatic eco-toxicity, and human toxicity.

## 2. Life cycle assessment methodology

Life cycle assessment (LCA) is a technique that helps investigate the environmental impact of a product from raw material extraction to disposal or recycling systematically [15]. This is achieved by quantifying all materials and energy inputs as well as waste and pollutants outputs enabling the comparison of the impacts of products manufactured and used for the same purpose. The present LCA study was performed according to the international standards, ISO 14040 [16] and ISO 14044 [17], although not being reviewed by an outside party.

The LCA framework methodology outlines four distinct stages: (1) goal and scope definition, (2) inventory analysis, (3) impact assessment and (4) interpretation. These stages should include all inputs and outputs needed to sufficiently conduct the LCA. The LCA performed in this paper was carried out considering all phases from raw material extraction to the production gate, following a cradle to gate assessment given that a) the majority of environmental impact is associated with the manufacturing stage of PV cells [18], and b) due to the emerging nature of the technologies the uncertainties associated with the use phase and end of life stages could be avoided in the LCA models.

### 2.1. Goal and scope definition

The environmental impacts of producing six inorganic chalcogenide thin film PV cells were evaluated in this study. The cells assessed included five emerging second-generation PV cells (CZTS, CZTSe, CZGeSe,  $Sb_2Se_3$  and  $Sb_2S_3$ ) and the commercially available CIGS cell, which was used as the reference technology. An LCA including materials for both the substrate and active layers of the solar cells alongside process auxiliaries such as water and electricity was performed.

Inventory data for the production of these cells were obtained from reputable manufacturers with impact assessment conducted using the GaBi LCA software (GaBi ts 9.2). The functional unit (FU) used in this study was 1 kWh of energy generated over the full lifetime of the cell. This FU was selected to provide a common basis for comparison between the different technologies with different efficiencies. The assessment followed a cradle to gate approach, accounting for all the impacts occurring from raw material extraction to the production gate. A cradle to gate approach was selected because majority of the technologies assessed in this study have not been deployed commercially and there is a lack of information of their end of life. Hence, data for the environmental assessment of the use phase could not be verified. Table 3 shows the efficiencies used to calculate the respective needed cell areas required to produce the functional unit (1 kWh). The area was calculated using the average solar radiation of the UK, which is 850 kWh/m<sup>2</sup> [19]. However, as this is a comparative assessment, results would be independent of the location used. Given that the assessed technology is not commercially available at this stage, an expected operational lifetime of 30 years and a performance ratio of 80% were assumed in this study in line with the international energy agency recommendations [20] to reduce uncertainty.

Fig. 1 demonstrates the system boundary detailing a cradle to gate analysis. It consists of only the manufacturing stage of cell production starting with raw material extraction, which are processed and used in cell assembly. Manufacturing of the PV cells consumes energy and other utilities alongside generating emissions; these are all accounted for in this study. The use and end of life phases of the cells were not considered in the system boundary. This is because it has been shown that the majority of environmental impact of PV cells comes from the manufacturing phase with this type of system boundary being applied to numerous LCA studies on PV technologies [18].

### 2.2. Life cycle inventory

Life cycle inventory quantifies the energy and raw material inputs for the manufacturing of the selected PV cells. All layers (insulation layer, back contact, buffer layer, and front contact) except the absorber are the same for each of the analysed cells with the kesterite-based cells making use of abundant earth mineral. This device architecture originally seen in CIGS solar cells does not cause any reduction in device performance when kesterite based absorbers are deployed [21]. Life cycle inventory data for the reference technology, CIGS cell, is shown in Table 4 and it takes into account all the steps involved in the manufacturing of the cell. These steps correspond to layer depositions of material that has specific functions on the cell. Stainless steel foil was used as the substrate and therefore the first layer of the cell. It was washed and then etched with a solvent which was assumed to be 1 M isopropanol [22]. An insulation layer with a thickness 0.3 μm was assumed to be then deposited by sputtering silicon oxide directly on the stainless steel substrate [23]. The back contact was made up of molybdenum with the CIGS absorber having a density and thickness of 5.7 g/cm<sup>3</sup> and 1 μm respectively [24]. This was used to calculate the inventory of its constituent metals. The environmental impacts of indium, gallium and selenium used in the absorber were calculated using an economic allocation method described in the work of Nuss and Eckelman where the five year average

Table 3

Efficiencies considered, and area required producing 1 KWh of energy for the assessed PV technologies.

S/N	Technology	Efficiency (%)	Area (cm <sup>2</sup> )	Reference
1	CIGS	20	2.45	[58]
2	CZTS	11	4.46	[11]
3	CZTSe	11.6	4.23	
4	CZGeSe	7.6	6.45	
5	$Sb_2Se_3$	7.6	6.45	
6	$Sb_2S_3$	7.6	6.45	

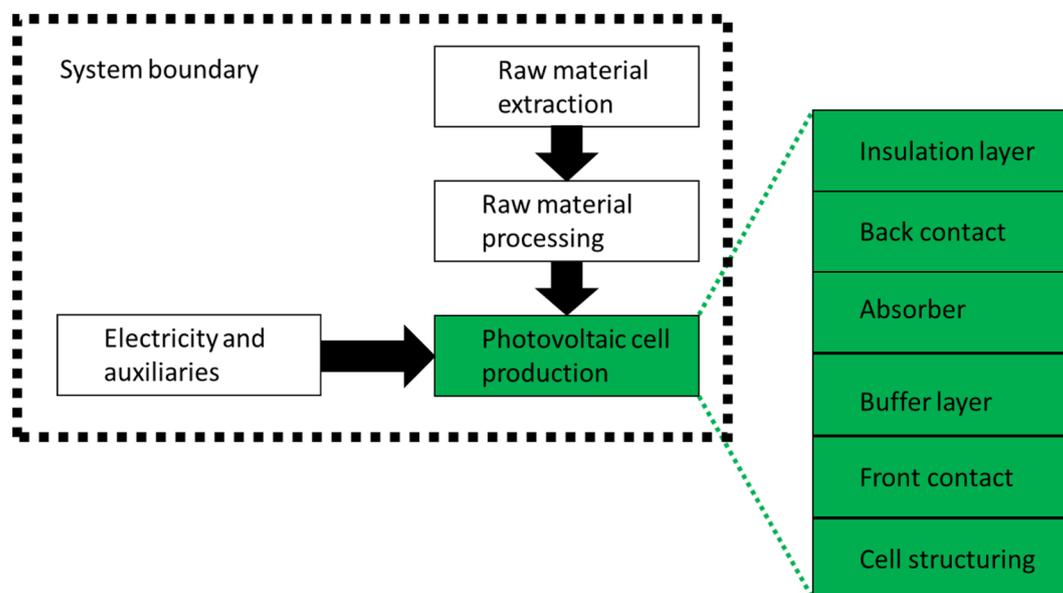


Fig. 1. System boundary for the life cycle assessment of the photovoltaic cells analysed (The green box indicate the manufacturing stages of producing the assessed PV cells).

Table 4

Life cycle inventory of the production of CIGS cells capable of producing 1 KWh of energy (Compiled by authors using manufacturer data).

	Input/Output	Amount	Unit
Cleaning	Detergent	1.2250	mg
	Water	1.2250	ml
	Electricity	0.0005	KWh
	Emissions- Detergent	1.2250	mg
	Emissions- Wastewater	1.2250	mg
Insulation Layer	Stainless steel foil	71.0500	mg
	Silicon-oxide powder	3846.5	mg
	Solvent (isopropanol)	0.0490	ml
	Electricity	0.0078	KWh
Back contact	molybdenum	2.0384	mg
	Sodium molybdate	0.1029	mg
	Cooling water	4.9000	ml
	Electricity	0.0042	KWh
Absorber	Copper	0.1181	mg
	Indium	0.1936	mg
	Gallium	0.0470	mg
	Selenium	0.3396	mg
	Cooling water	7.3500	ml/min
	Electricity	0.0451	KWh
Buffer layer	Cadmium acetate	1.2985	mg
	Ammonia	0.0065	ml
	Thiourea	1.0290	mg
	Deionised water for reaction	3.2585	ml
	Cooling water	4.9000	ml/min
	Electricity	0.0023	KWh
Front Contact	Indium	0.1911	mg
	Oxygen	0.0064	mg
	Tin	0.0216	mg
	Cooling water	7.3500	ml/min
	Electricity	0.0007	KWh
Cell Structuring	Cooling water	3.6750	ml/min
	Electricity	0.0032	KWh
Printing interconnection	Printing inks	0.0015	ml
	Electricity	0.0039	KWh
Auxiliary products	Helium	0.0061	ml
	Oxygen	0.6125	ml
	Argon	7.1050	ml

market price of the metals was used due to lack of data [25]. These market prices (2016–2020) for indium, gallium and selenium were obtained from the United States Geological Survey database [26]. Indium is produced from the processing of zinc while gallium and selenium from

alumina and copper processing respectively, this was used as the basis for the economic allocation [25]. A density and thickness of  $7.14 \text{ g/cm}^3$  and  $0.25 \mu\text{m}$  was used for the front contact [24]. It was assumed that only 20 percent of the sputtering materials make it to the insulation layer, absorber and front contact with the excess input treated as hazardous waste deposited directly into the atmosphere in this cradle to gate study [27]. Cadmium acetate was used as the buffer layer although zinc oxy-sulfide is being investigated as an alternative due to the potentially toxic nature of cadmium [28]. Life cycle inventory data for the printing ink used for monolithic interconnection of cells was taken from the work of Fernandes and co-workers [29]. Silver nanoparticles conductive ink was selected here because it does not degrade the performance of solar cells unlike other metal inks [30]. The ink was assumed to be made up of 8 wt% silver nanoparticles and ethanol which acted as the solvent [29]. Electricity and other auxiliary products were assumed to be supplied from the average of the 28 countries in the European Union (EU-28) from the database of GaBi.

Table 5 demonstrates the inventory data for the absorber layer of the five other types of chalcogenide PV cells assessed. All the other layers including insulation layer, back contact, buffer layer, and front contact, alongside all system assumptions remain the same as the reference technology (CIGS PV cell) described above (see Appendix A1–A5 for full life cycle inventory of CZTS, CZTSe, CZGeSe,  $\text{Sb}_2\text{Se}_3$ ,  $\text{Sb}_2\text{S}_3$ ).

### 2.3. Life cycle impact assessment

Thirteen impact categories were selected from the CML 2001 [31] impact characterisation and cumulative energy demand (CED) [32] methods (see Table 6). These categories included abiotic depletion (ADP), abiotic depletion (fossil fuels) (ADPF), global warming potential (GWP), ozone layer depletion (ODP), human toxicity (HT), freshwater aquatic eco-toxicity (FWE), marine aquatic eco-toxicity (MAE), terrestrial eco-toxicity (TE), photochemical oxidation (POP), acidification (AP), eutrophication (EP), primary energy non-renewable resource (PENRT) and primary energy renewable resource (PERT). The GWP is considered the most important environmental impact category of the thirteen selected as it indicates whether the manufactured solar cell actually helps in mitigating climate change. However, it is crucial to assess other impact categories to ensure that mitigating global warming does not unintentionally transfer environmental burdens to other impact categories.

**Table 5**

Life cycle inventory data for the absorber layers of the selected chalcogenide photovoltaic cells capable of producing 1 KWh of energy (compiled by authors using manufacturer data).

S/N	Absorber type	Input/ Output	Amount	Unit
1	Cu <sub>2</sub> ZnSnS <sub>4</sub>	Copper	0.8913	mg
		Zinc	0.4456	mg
		Tin	0.8244	mg
		Sulphur	0.8913	mg
		Electricity	0.0486	KWh
		Argon	1114.0820	ml
2	Cu <sub>2</sub> ZnSnSe <sub>4</sub>	Waste - Sulphur	16.9340	mg
		Copper	0.5916	mg
		Zinc	0.2958	mg
		Tin	0.5494	mg
		Selenium	1.4368	mg
		Electricity	0.0461	KWh
3	Cu <sub>2</sub> ZnGeSe <sub>4</sub>	Argon	845.1657	ml
		Waste - Selenium	27.2989	mg
		Copper	0.9030	mg
		Zinc	0.4515	mg
		Germanium	0.5805	mg
		Selenium	2.1930	mg
4	Sb <sub>2</sub> Se <sub>3</sub>	Electricity	0.0703	KWh
		Argon	1289.9897	ml
		Waste - Selenium	41.6667	mg
		Antimony	1.5480	mg
		Selenium	1.4835	mg
		Electricity	0.0387	KWh
5	Sb <sub>2</sub> S <sub>3</sub>	Argon	1612.4871	ml
		Waste - Selenium	12.8999	mg
		Antimony	1.0578	mg
		Sulphur	0.4128	mg
		Electricity	0.0387	KWh
		Argon	1612.4871	ml
		Waste - Sulphur	7.7399	mg

**Table 6**

Impact categories assessed with the CML 2001 and cumulative energy demand method with their abbreviations and unit [31,32].

Category	Abbreviation	Unit	Method
Abiotic depletion	ADP	Kg Sb eq	CML 2001
Abiotic depletion (fossil fuels)	ADPF	MJ	
Global warming	GWP	Kg CO <sub>2</sub> eq	
Ozone layer depletion	ODP	Kg CFC-11 eq	
Human toxicity	HT	Kg 1,4-DB eq	
Fresh water aquatic eco-toxicity	FWE	Kg 1,4-DB eq	
Marine aquatic eco-toxicity	MAE	Kg 1,4-DB eq	
Terrestrial eco-toxicity	TE	Kg 1,4-DB eq	
Photochemical oxidation	POP	Kg C <sub>2</sub> H <sub>4</sub> eq	
Acidification	AP	Kg SO <sub>2</sub> eq	
Eutrophication	EP	Kg PO <sub>4</sub> eq	
Primary energy non-renewable resource	PENRT	MJ	Cumulative energy demand
Primary energy renewable resource	PERT	MJ	

Energy generation is the primary purpose of PV cells; therefore, it is essential to know the amount of energy invested to obtain energy production from the cells. This can be assessed using cumulative energy demand method as it gives the total energy used for its cradle to gate production considering both renewable and non-renewable energy sources. Alongside energy utilisation, metal production is also a major environmental issue of the reference technology (CIGS cell). Therefore, it was important that the assessment included the abiotic depletion of

these resources hence why the CML 2001 characterisation method was chosen. Normalisation of the results associated with the CML 2001 impact method was also conducted using the CML 2001 –Jan 2016, EU25 + 3 factors found in GaBi.

## 2.4. Sensitivity analysis

A sensitivity analysis using the ILCD 2011 [33] and IMPACT 2002+ [34] characterisation methods was also conducted. These methods alongside the CML 2001 method are highly relevant when assessment of metal depletion is being considered. The objective of the sensitivity analysis was to compare the effects of using different LCA characterisation methods on environmental impact results of the thin film PV cells assessed. Table 7 and Table 8 demonstrate the impact categories for the ILCD 2011 and IMPACT 2002+ methods, respectively.

## 3. Results and discussion

### 3.1. Environmental impact of CIGS solar cell

The following sections present the environmental impact assessment of CIGS cells as a commercially available technology and use the results as a benchmarking point for the emerging technologies that are being investigated in this paper. The materials and processes contributing to the dominant impact categories are identified in order to assist the manufacturers in exploiting the results of the analyses.

#### 3.1.1. Impacts from materials and energy

By combining the considered process model assumptions, life cycle inventories and characterisation factors of the CML 2001 method, the environmental impact profiles of the selected impact categories for CIGS were calculated. Table 9 demonstrates the environmental impact results of electricity consumption, materials, and chemicals used to manufacture the cell in relation to the defined functional unit.

The results displayed in Table 9 indicate that electricity consumption has the highest impact in ten (ADPF, GWP, FWE, MAE, TE, POP, AP, EP, PENRT and PERT) of the selected impact categories, while materials used had relatively high impact in three other categories (ADP, ODP and HT).

The high environmental impact for materials used in the ADP and ODP is due to the use of molybdenum as the back contact with the metal contributing 14.5% of ADP and 96.7% of ODP respectively. As for the

**Table 7**

Impact categories assessed with the ILCD 2011 midpoint characterization method [33].

S/ N	Category	Abbreviation	Unit	Method
1	Climate change	CC	kg CO <sub>2</sub> eq	ILCD
2	Ozone depletion	OD	kg CFC-11 eq	2011
3	Human toxicity, non-cancer effects	HTnc	CTUh	
4	Human toxicity, cancer effects	HTc	CTUh	
5	Particulate matter	PM	kg PM2.5 eq	
6	Ionizing radiation HH	IR	kBq U235 eq	
7	Photochemical ozone formation	POF	kg NMVOC eq	
8	Acidification	AP	molc H + eq	
9	Terrestrial eutrophication	TEP	molc N eq	
10	Freshwater eutrophication	FEP	kg P eq	
11	Marine eutrophication	MEP	kg N eq	
12	Freshwater eco-toxicity	FWE	CTUe	
13	Land use	LU	kg C deficit	
14	Water resource depletion	WRD	m <sup>3</sup> water eq	
15	Mineral, fossil and resource depletion	MFRD	kg Sb eq	

**Table 8**  
Impact categories assessed with the IMPACT 2002+ characterization method [33]

S/N	Category	Abbreviation	Unit	Method
1	Carcinogens	CA	kg C <sub>2</sub> H <sub>3</sub> Cl eq	IMPACT 2002+
2	Non carcinogens	NC	kg C <sub>2</sub> H <sub>3</sub> Cl eq	
3	Respiratory inorganics	RE	kg PM2.5 eq	
4	Ionizing radiation	IR	Bq C-14 eq	
5	Ozone layer depletion	OD	kg CFC-11 eq	
6	Aquatic eco-toxicity	AE	kg TEG water	
7	Terrestrial eco-toxicity	TE	kg TEG soil	
8	Terrestrial acid/nitrification	TA	kg SO <sub>2</sub> eq	
9	Land occupation	LO	m <sup>2</sup> org. arable	
10	Aquatic acidification	AA	kg SO <sub>2</sub> eq	
11	Aquatic eutrophication	AEP	kg PO <sub>4</sub> P-lim	
12	Global warming	GW	kg CO <sub>2</sub> eq	
13	Non-renewable energy	NRE	MJ primary	
14	Mineral extraction	ME	MJ surplus	

**Table 9**  
Life cycle impact assessment results for CIGS Cell (impact per kWh).

Impact Category	Unit	CIGS			
		Electricity	Materials	Chemicals	Others
ADP	Kg Sb eq	9.00E-09	1.20E-07	1.31E-07	7.38E-11
ADPF	MJ	3.00E-01	3.05E-03	2.70E-03	9.13E-05
GWP	Kg CO <sub>2</sub> eq	2.67E-02	2.62E-04	1.12E-04	7.01E-06
ODP	Kg CFC-11 eq	8.60E-16	2.55E-14	4.14E-18	1.80E-19
HT	Kg 1,4-DB eq	1.17E-03	6.09E-03	1.47E-05	2.96E-07
FWE	Kg 1,4-DB eq	5.87E-05	1.25E-05	1.01E-06	4.44E-08
MAE	Kg 1,4-DB eq	3.13E+00	9.10E-02	1.11E-02	6.09E-04
TE	Kg 1,4-DB eq	3.12E-05	1.97E-06	8.28E-07	3.28E-08
POP	Kg C <sub>2</sub> H <sub>4</sub> eq	3.80E-06	7.64E-08	4.08E-08	1.14E-09
AP	Kg SO <sub>2</sub> eq	4.93E-05	1.49E-06	3.54E-07	1.33E-08
EP	Kg PO <sub>4</sub> eq	6.16E-06	7.84E-08	2.56E-08	4.35E-09
PENRT	MJ	5.07E-01	3.61E-03	3.05E-03	1.24E-04
PERT	MJ	2.21E-01	7.08E-04	1.81E-04	3.98E-05

HT impact category, stainless steel use in the insulation layer is responsible for around 80% of this impact. Chemicals consumed in the manufacturing of the CIGS cell contributed significantly (50.4%) to the ADP impact category, similar to the 46.1% that was attributed to materials used. The chemical responsible for such high levels of impact in the ADP category is cadmium acetate used in the buffer layer as it contributed 83.7% to the category when only chemicals consumed are taken into account.

The overall contribution to climate change of the CIGS cell (around 98% of the GWP) is mainly due to electricity consumption. This GWP contribution is similar to what was seen by Collier and co-researchers where a similar cradle to gate analysis was conducted on CIGS cell [18]. Alongside global warming, other environmental indicators such as eco-toxicity are aligned with those obtained in Collier's study.

### 3.1.2. Impacts from each manufacturing stage

The environmental impact for each manufacturing step alongside printing interconnection and auxiliary materials used to produce the

assessed CIGS solar cell are detailed in Fig. 2. The absorber was found to have the highest impact for almost all the selected impact categories. It was also a significant contributor to the ADP (30.6%) and HT (10.7%) impact categories.

Alongside the absorber, the buffer layer is also a significant contributor to the ADP (42.2%) impact category due to the use of cadmium acetate. However, this layer does not considerably affect other impact categories as it was always < 5% in the remaining categories due to the limited contribution of cadmium acetate.

The analysis of the back contact revealed that it was the major contributor (96.9%) to the OD impact category due to the use of molybdenum. It was also prominent in other categories. The relatively low impact in HT is due to 83.7% of the impact coming from the use of stainless steel in the insulation layer. The insulation layer was also significant in ten other impact categories (ADPF, GWP, FWE, MAE, TE, POP, AP, EP, PENRT, PERT), recording more than 10% in each of them.

The process of printing interconnection contributed to around 7% of the ADPF, GWP, FWE, MAE, TE, POP, AP, EP, PENRT and PERT impact categories with most of the impact coming from electricity (0.0039 KWh) used in the process. Substrate cleaning, front contact and use of auxiliary materials such as helium, oxygen and argon did not significantly affect the overall impact of the CIGS cell, as the main hotspots of the manufacturing process are the absorber, insulation layer, back contact and buffer layer.

### 3.2. Comparison of the environmental impact of emerging chalcogenides thin film solar cells

The environmental impacts of the emerging chalcogenide solar cells are presented in the following sections. The results are categorised into materials and energy, and the manufacturing stages. Similar to the previous sections, the main contributing materials and processes are highlighted to enhance the effectiveness of the analyses. Where relevant, the results are analysed to highlight their implications for different stakeholders.

#### 3.2.1. Impacts from materials and energy

The results indicated that as with the CIGS cell (see Table 9) electricity consumption has the highest impact in most of the categories. The environmental impact results of electricity consumption, materials, and chemicals used to manufacture CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> demonstrated in general a similar trend to the CIGS values and are further detailed in the Supplementary Materials (see Appendix B1–B5).

The chemicals contributed significantly to the ADP impact category for the CZTS cell due to its absorber layer having a comparatively low impact in this category. Results obtained here for CZTS align with those observed by Collier and co-researchers [18].

Overall, the impacts of CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> were seen to be higher than CIGS for electricity, materials and chemicals used in all the selected impact categories. This is mainly attributed to the lower efficiency of the cells, which in turn led them to be larger than the CIGS cell in area. The electricity required to manufacture CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> cells per functional unit, was 37%, 30%, 98%, 55% and 55% higher than that needed for CIGS, respectively.

The results suggest that reducing the electricity consumption in the manufacturing stages and/or improvements made over minimising the grid carbon intensity could significantly reduce the environmental impact of thin-film technologies in general given the smaller quantity of materials being used for their manufacturing. The analyses also suggest that for the emerging technologies to compete with established commercially available technologies, higher efficiencies need to be targeted.

#### 3.2.2. Impacts from each manufacturing stage

The environmental impact for each manufacturing step alongside printing interconnection and auxiliary materials used to produce CZTS,

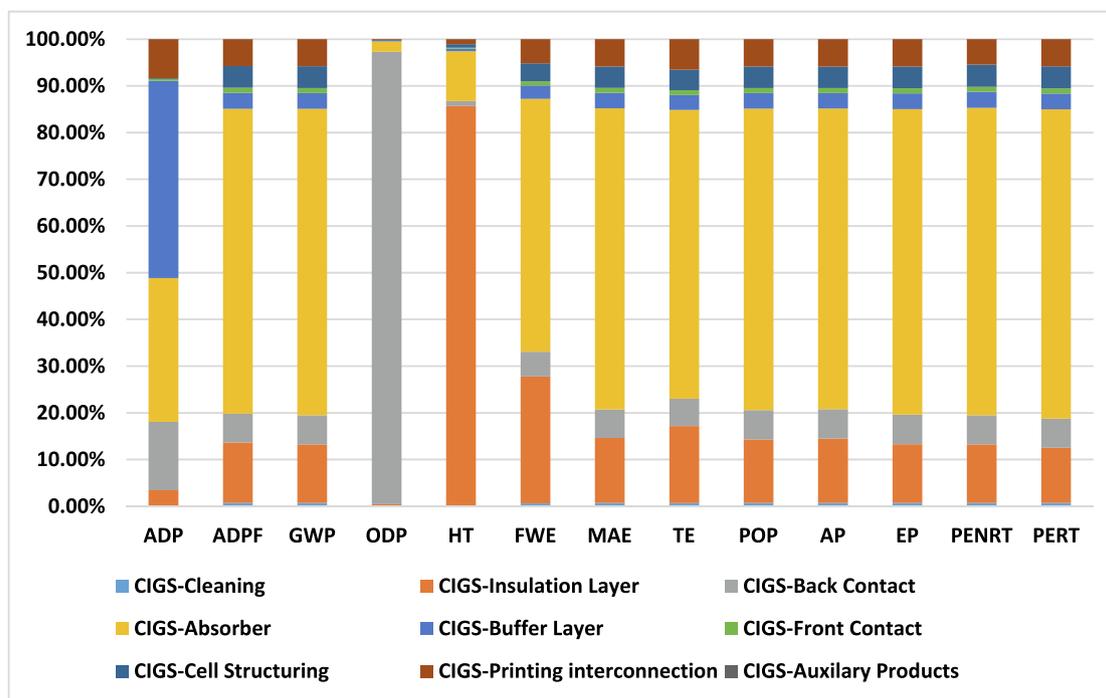


Fig. 2. Contribution to impact categories for the production of CIGS (impact per KWh).

CZTSe, CZGeSe,  $\text{Sb}_2\text{Se}_3$  and  $\text{Sb}_2\text{S}_3$  are detailed in Fig. 3. For all five technologies as with CIGS, it was observed that the absorber has the highest impact in majority of the selected impact categories. Comparing the environmental impact of the manufacturing steps of the CIGS to that of the other analysed cells suggests that a shift to the inorganic cells (CZTS, CZTSe, CZGeSe,  $\text{Sb}_2\text{Se}_3$  and  $\text{Sb}_2\text{S}_3$ ) led to a decrease in the overall contribution of the absorber in the majority of the impact categories. This is attributed to the CIGS absorber consuming more electricity compared to the other cells.

There was a decrease on average of 10.46% in CZTS, 8.66% in CZTSe, 8.65% in CZGeSe, 22.44% in  $\text{Sb}_2\text{Se}_3$  and 21.34% in  $\text{Sb}_2\text{S}_3$  to the overall contribution of the absorber when there was a shift away from CIGS. The CZTSe, CZGeSe,  $\text{Sb}_2\text{Se}_3$  and  $\text{Sb}_2\text{S}_3$  absorbers contributed to over 80% of the ADP impact category. This is due to the use of more materials for absorber layering than those of CIGS and CZTS. The main hotspot of the manufacturing processes is the absorber layer. Improved efficiencies for CZTS, CZTSe, CZGeSe,  $\text{Sb}_2\text{Se}_3$  and  $\text{Sb}_2\text{S}_3$  are required in order to see the discussed environmental benefits over the highly efficient CIGS cells.

### 3.3. Comparative analysis of CIGS and chalcogenides thin film solar cells

The same environmental indicators of the CML 2001 method were used to compare the CIGS results with five other chalcogenides thin film solar cell assessed considering current efficiencies. Fig. 4 displays the results obtained relative to the maximum in each of the selected impact categories based on the efficiencies presented in Table 3.

CIGS was always < 55% of the maximum in all categories and it was mainly due to the lower electricity needed to produce the CIGS cell ( $2.45 \text{ cm}^2$ ) capable of generating the functional unit (1 KWh), given its higher efficiency. The absorber area for the same electricity generation capacity is  $4.46 \text{ cm}^2$  for CZTS and  $4.23 \text{ cm}^2$  for CZTSe relative to their lower associated efficiencies.

The antimony-based cells ( $\text{Sb}_2\text{Se}_3$  and  $\text{Sb}_2\text{S}_3$ ) had the second highest impact in the GWP, ODP, HT, FWE, MAE, TE, POP, AP, EP, PENRT and PERT always greater than 60% to the maximum. They were comparable to the maximum, which was CZGeSe, in the ODP and HT impact categories. This was due to same amount of molybdenum and stainless steel

being used to manufacture the cells (CZGeSe,  $\text{Sb}_2\text{Se}_3$  and  $\text{Sb}_2\text{S}_3$ ). Assessing the kesterite based cells (CZTS and CZTSe), for all the impact categories except the ADP, similar impacts were observed. This, as with the antimony based cells ( $\text{Sb}_2\text{Se}_3$  and  $\text{Sb}_2\text{S}_3$ ), is due to them having the same efficiency and hence similar area needed to produce the functional unit.

Looking specifically at the ADP impact category, the cells with the lowest impact were the CIGS and CZTS, with <5% of the maximum.  $\text{Sb}_2\text{S}_3$  can also be seen to be relatively low in this category (ADP) due to the use of lower quantities of raw materials such as antimony and selenium with high impacts on ADP.

The categories presented in impact assessment methods in general have different units, making a direct comparison between the impact categories more challenging. In order to facilitate easier interpretation of results a normalisation study has been performed to assess all the impact categories and express them using the same units, benefiting non-expert stakeholders [35].

Fig. 5A demonstrates the normalised values relative to each impact category for the assessed technologies while Fig. 5B displays the total normalised environmental impact score for the cells.

For the majority of the cells, the impact category MAE has the greatest contribution (48.6 – 66.3% of the total contribution). MAE estimates the environmental impact of harmful chemicals on marine ecosystem and it is mainly caused by fluoride emissions from electricity production [36].

ADP and HT were the other impact categories that had significant contribution in majority of the analysed cells. The majority of the impact in HT comes from stainless steel in the insulation layer of the cells. In general, for all the assessed cells the impact categories ODP, FWE, TE and EP had negligible normalisation environmental impact. Assessing the ADP impact category, it is evident that CZTS and CIGS absorbers were seen to have relatively low environmental impact, with CZTSe, CZGeSe and  $\text{Sb}_2\text{Se}_3$  displaying high relative values. This was attributed to the amount of Se needed to manufacture these absorbers. CZTSe and CZGeSe require 28.7 mg and 43.9 mg of Se, respectively with only 5% making it to the absorber [37,38]. This is also the case for  $\text{Sb}_2\text{Se}_3$  (14.4 mg of Se) as around 90% excess Se does not make it to the absorber. The metal (Se) contributed a significantly to ADP for the absorbers of CZTSe,

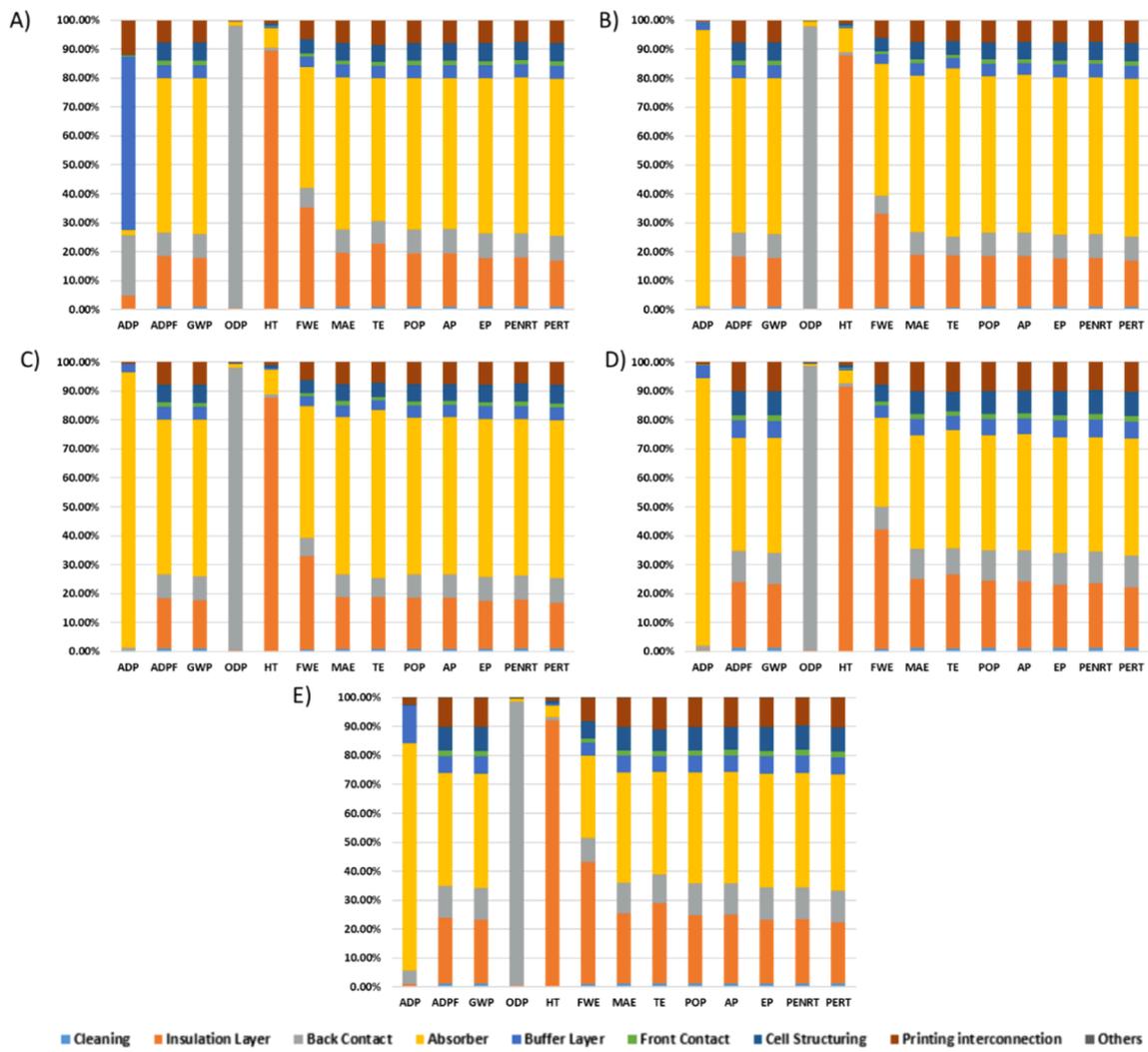


Fig. 3. Contribution to impact categories for the production of A) CZTS B) CZTSe C) CZGeSe D) Sb<sub>2</sub>Se<sub>3</sub> and E) Sb<sub>2</sub>S<sub>3</sub> (impact per kWh).

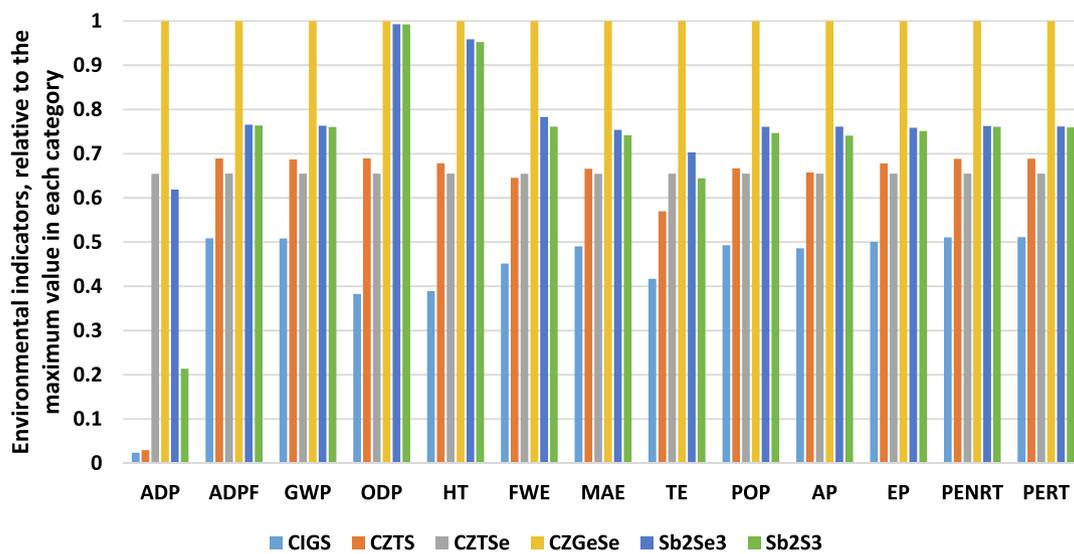


Fig. 4. Life cycle impact assessment results for CIGS, CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> calculated using CML 2001 (results are displayed relative to the maximum).

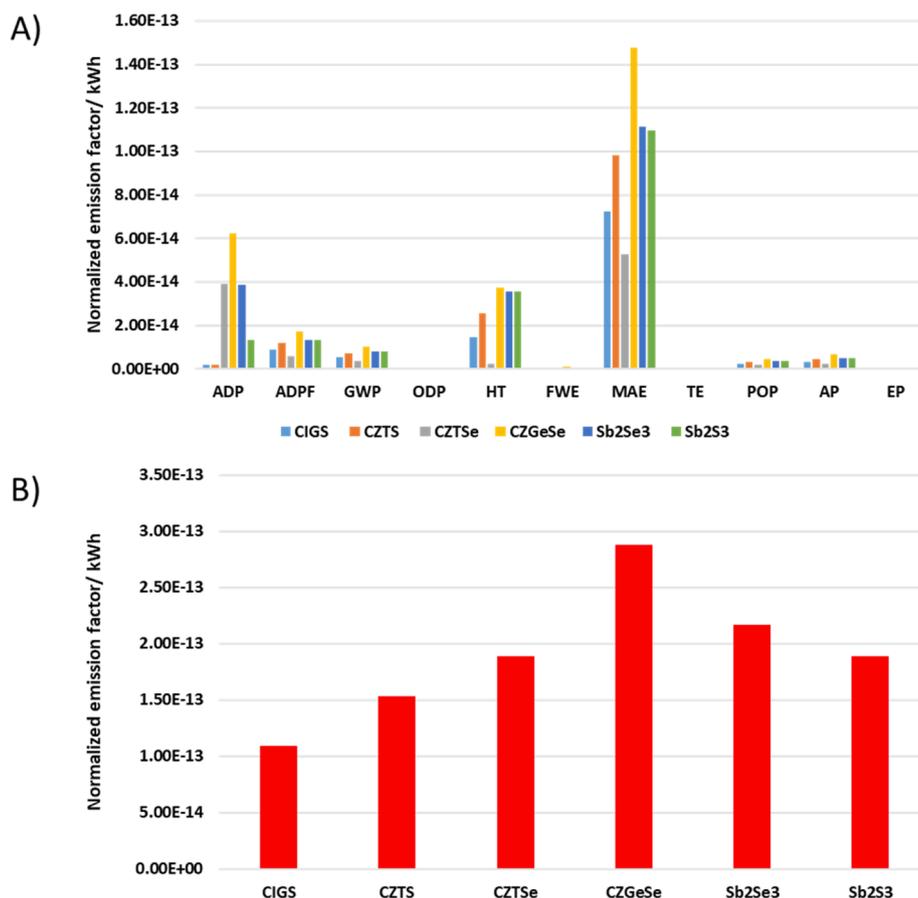


Fig. 5. Normalised emission factor for the assessed chalcogenide thin film solar cells A) Environmental impact category B) Total individual cell score.

CZGeSe, and Sb<sub>2</sub>Se<sub>3</sub>.

Comparing the total normalisation score of the assessed cells (Fig. 5B) demonstrates that CZGeSe had the highest score because it having the most energy intensive manufacturing process while CIGS had the lowest. This was expected as they both had the highest and lowest impact respectively in all the selected impact categories (see Fig. 4).

### 3.4. Sensitivity analysis

#### 3.4.1. Impact characterisation method analysis

LCA results may be affected by the impact characterisation method selected in the study. Hence, a sensitivity analysis was conducted using other relevant characterisation methods. For this analysis, the ILCD 2011 and Impact 2002+ characterisation methods were selected. The ILCD 2011 was selected primarily due to having similar resource impact

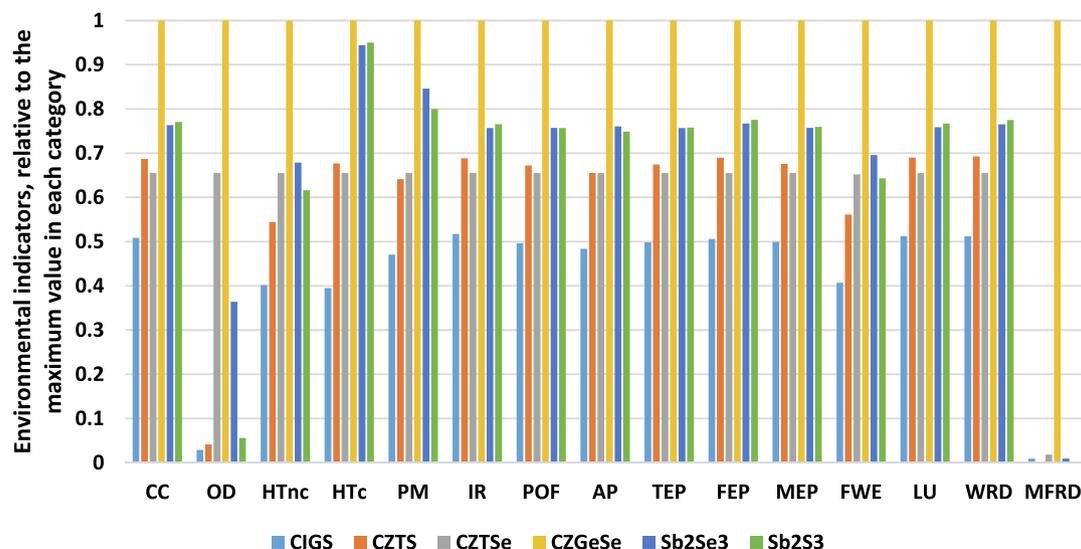


Fig. 6. Life cycle impact assessment results for CIGS, CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> calculated using ILCD 2011 (Results are displayed relative to the maximum).

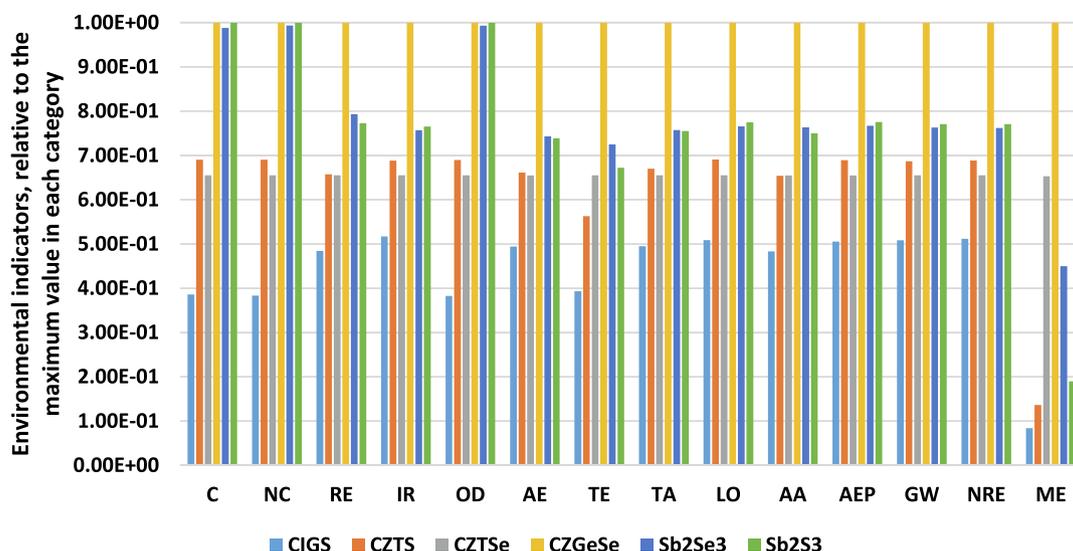


Fig. 7. Life cycle impact assessment results for CIGS, CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> calculated using IMPACT 2002+ (Results are displayed relative to the maximum).

assessment categories to the CML 2001. The ADP of the CML 2001 and MFRD of the ILCD are both measured in antimony equivalent. Alongside this the Impact 2002+ characterisation also has a similar unit to the CML 2001 method in the GWP (kg CO<sub>2</sub> eq) impact category.

Fig. 6 and Fig. 7 demonstrate the results for the ILCD 2011 and IMPACT 2002+ impact characterisation methods, respectively. It can be observed that using these characterisation methods, CZGeSe still has the highest environmental impact in most of the impact categories. CIGS recorded the lowest in almost all the impact categories for both methods.

CZGeSe in the MFRD impact category of the ILCD 2011 characterisation method (Fig. 6) demonstrates significantly higher values than CIGS and the other assessed cells. This is because germanium is used in its absorber layer. Germanium, gallium and indium used to manufacture CZGeSe and CIGS are on the European Union’s critical raw materials list and therefore have very high supply risk [39]. However, required germanium (0.5805 mg) in CZGeSe is in far greater quantities than the gallium (0.0470 mg) and indium (0.1936 mg) in CIGS.

The OD results demonstrate a difference between the ILCD2011 and CML 2001 methods in general. This is due to the discrepancies in the

impact of copper in the two methods with the ILCD 2011 being three orders of magnitude higher than values seen in the CML 2001 impact category. For example, for the CZTS cell, the ILCD 2011 calculated an impact of 3.85E-18 kg CFC-11 eq for copper while a value of 8.30E-14 kg CFC-11 eq was recorded in the CML 2001.

The values associated with impact 2002+ method follows the same trend as the CML 2001 method for all indicators. However, values are a percentage point lower than in the CML 2001. The sensitivity study on the characterisation methods highlights that there is no consensus between the studied methods concerning the impact on resources and ozone depletion indicators due to differences in how the impact of copper is calculated. However, for all the other impact categories, the observed trend and associated causes are the same with CIGS having the lowest impact on the environment in majority of the selected impact categories due to its higher efficiency.

### 3.4.2. Efficiency analysis

The environmental impacts of studied PV cells were analysed considering a functional unit of 1KWh based on their current efficiencies

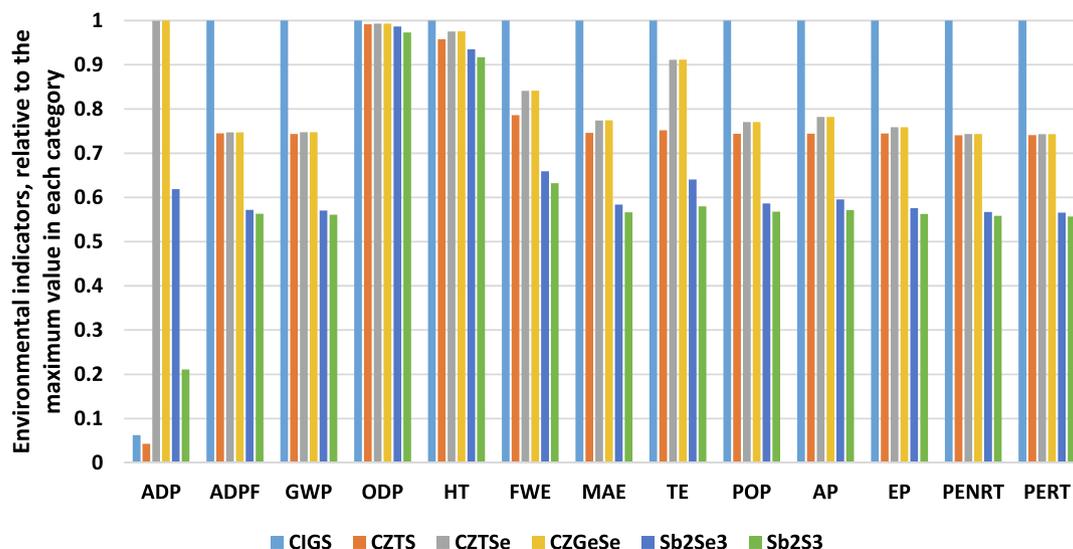


Fig. 8. Life cycle impact assessment results for CIGS, CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> when cell efficiency is 20% (Results are displayed relative to the maximum).

referenced in the literature. Fig. 8 however, displays the environmental impact of all six technologies assuming identical efficiencies of 20% allowing for a direct comparison between the technologies for a given scenario where the emerging technologies achieve equivalent efficiencies.

The analysis demonstrates better environmental outcome for the CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> cells. CIGS now has the highest impact in all impact categories except ADP. Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> were seen to have the least impact on the environment in these same categories. The ADP impact category followed the same trend as those observed at the different efficiencies with CZGeSe having the highest impact. However, unlike results in Fig. 4, CZTS has the lowest impact in this category (ADP).

Fig. 9 shows the normalised impact results assuming 20% efficiencies for all the cells. CIGS can be seen to now rival CZTSe and CZGeSe in the total normalisation score with CZTS, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> now having a lower score than the established technology. The sensitivity analysis and normalisation study reveal that if the efficiency of CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> cells can rival CIGS, there would be an environmental benefit to their deployment over the established CIGS technology.

Environmental impact results from this study were subsequently compared with other LCA studies assessing chalcogenide thin film solar cells. The comparison was done per meter square to eliminate the effects of efficiency. GWP and CED were used as proxies instead of the most significant impact categories MAE, HT and ADP as they are the most commonly used environmental indicators in the previous LCA studies. Table 10 indicate that when the effects of efficiencies are eliminated emerging chalcogenide thin film solar cells such as CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> have the ability to rival the already established cells, CIGS and CIS, in terms of their environmental performance. This improved performance could pave a pathway to their deployment as researchers strive to improve the efficiencies of these emerging cells.

#### 4. Conclusions

The calculation of the environmental impact of emerging chalcogenide thin film PV cells using primary manufacturer data, for the first time, allowed for a comprehensive study on how these technologies compared with the commercially available CIGS. Results demonstrated that the environmental performance of these cells are sensitive to changes in efficiency. In order to be able to interpret the results more

**Table 10**

Comparison of the GWP and CED of life cycle assessment studies on chalcogenide thin film solar cells.

Cell Type	Efficiency (%)	GWP (Kg CO <sub>2</sub> eq/m <sup>2</sup> )	CED (MJ/m <sup>2</sup> )	References
CIGS	20	110.59	3005	This study
CZTS	11	82.16	2226	
CZTSe	11.6	82.61	2233	
CZGeSe	7.6	82.62	2234	
Sb <sub>2</sub> Se <sub>3</sub>	7.6	63.08	1703	
Sb <sub>2</sub> S <sub>3</sub>	7.6	62.84	1699	
CIGS	10.5	65	1936	[41]
	12	62.76	1248	[59]
	12	91.92	1236	
	15	34.5	-	[55]
CIS	11	52.42	1117	[46]
	11	201	1234	[47]
	11	266.5	4334	[52]
	11	196.35	3047	
CZTS	10	145.35	-	[18]
	15	4.57	-	[57]
	15	0.57	-	

effectively, a comprehensive normalisation study of environmental impact results was conducted. The normalisation study clearly highlighted that at current efficiency levels, CIGS performs better than the others due to less production materials and energy required to manufacture the same amount of electricity over the cells' lifetime, suggesting that for any emerging technology to be able to compete with commercially established solar technologies, higher/equivalent efficiencies need to be achieved.

The normalisation study and the results analysed through the impact assessment methods, identified the relevant environmental hotspots. Such identifications could be used by product developers and manufacturers to, where necessary, replace materials and chemicals with environmentally friendlier alternatives. For example, zinc-based alternatives to cadmium acetate such as zinc oxysulfide could be used in the buffer layer to reduce their associated environmental impact. Stainless steel in the insulation layer and molybdenum in the back contact contributed significantly to the toxicity and ozone depletion impact categories for all cells assessed and their use could be scrutinised further. The analysis also suggested that the absorber layers are the most demanding manufacturing stage, contributing the most to majority of the impact categories assessed. This is due to the absorber layer

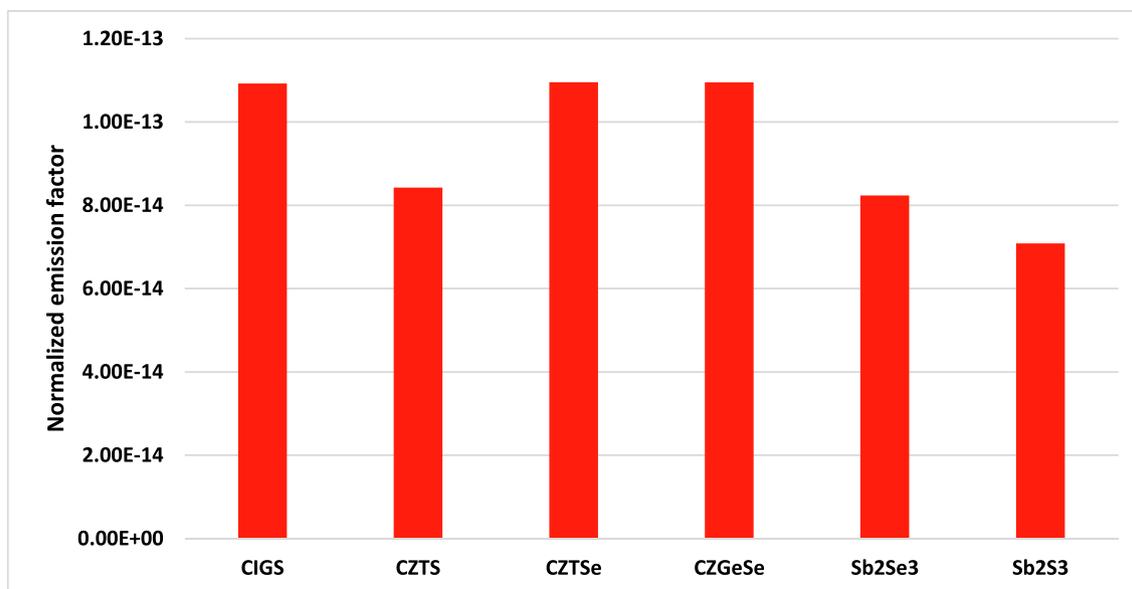


Fig. 9. Normalised emission factor for the assessed chalcogenide thin film solar cell when cell efficiency is 20%

requiring the most electricity to produce, significantly affecting the impact attributed to it in all the assessed impact categories except abiotic depletion. The electricity consumed in the manufacturing process was found to be the main hotspot of thin film PV cell production. Solutions such as grid decarbonisation would improve impact results greatly. The elements selenium and antimony found in all assessed emerging chalcogenide absorbers (CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub>) except CZTS contributed considerably to the abiotic depletion impact category of the absorber layers. A switch from CIGS to other analysed chalcogenide cells were found to reduce the overall impact of the absorber layer. This is important as it indicates that the environmental impact of producing the same size of the other emerging chalcogenide cells could rival CIGS.

A sensitivity analysis was conducted in this study, assuming similar efficiencies leading to the same required cell area. The normalised results indicate that if efficiencies of the other cells (CZTS, CZTSe, CZGeSe, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub>) were comparable to CIGS, there would be an environmental benefit of deploying CZTS, Sb<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>S<sub>3</sub> over the commercially available CIGS as it now had similar impact to CZTSe and CZGeSe. This further highlights the significance of the research currently being undertaken to improve the efficiency of the emerging solar cells.

Recycling cell materials at the end of life could also contribute greatly to reducing the associated impact through extending the lifetime of the materials and keeping them in the cycle of use for longer. However, recycling can be problematic as the quantity of materials that can be recovered from thin film solar cells at end of life is low and economically unattractive. Nevertheless, the environmental benefit of recycling high value materials should be carefully considered. The presented results could be also relevant to assess how these technologies can be designed with the environment in mind rather than seeking solutions as an afterthought.

Given the emerging nature of the technologies investigated, a cradle to gate system boundary was adopted in this study to minimise the uncertainties in the LCA analysis. Future research however, could expand the system boundaries to include all the relevant scenarios for the use phase and the end-of-life stages to provide a more comprehensive analysis for the relevant end-users of the findings.

It is also worth noting that the application of LCA as a decision making tool is heavily reliant on the availability of accurate, reliable, and high-quality data. Gathering data with such qualities has proven difficult for LCA end users and practitioners due to a variety of reasons, including manufacturer confidentiality requirements, the time and expertise required to generate reliable data, and inconsistent application of methodological approaches to data analysis. Such challenges and barriers have limited the use of LCA as a decision making tool to primarily academic research. For the LCA studies to be used effectively as a decision making tool standardised and harmonised approaches need to be developed and implemented by the LCA community. The onus remains on LCA specialists and practitioners, as well as other key stakeholders, to harmonise the science across all relevant industries.

#### CRedit authorship contribution statement

**Shahaboddin Resalati:** Conceptualization, Methodology, Writing – review & editing, Supervision. **Tobechi Okoroafor:** Data curation, Writing – original draft, Software. **Amani Maalouf:** Methodology, Investigation. **Edgardo Saucedo:** Conceptualization, Validation. **Marcel Placidi:** Validation, Writing – review & editing.

#### Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Acknowledgments

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 952982. E.S. thanks European Union H2020 Framework Programme for the ERC Consolidator Grant under Grant Agreement no. 866018 (SENSATE). M.P. acknowledges the financial support from Spanish Ministry of Science, Innovation and Universities within the Ramon y Cajal program (RYC-2017-23758).

The authors would also like to express their gratitude to Bart Vermang, Sebastien Lizin, and Rajagopalan Neethi for their valuable comments and suggestions.

#### Appendix A. Supplementary material

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.apenergy.2022.118888>.

#### References

- [1] IRENA. Future of solar photovoltaic: deployment, investment, technology, grid integration, and socio-economic aspects. International Renewable Energy Agency; 2019.
- [2] Celik I, Song Z, Cimaroli AJ, Yan Y, Heben MJ, Apul D. Life Cycle Assessment (LCA) of perovskite PV cells projected from lab to fab. *Sol Energy Mater Sol Cells* 2016; 156:157–69.
- [3] Ibn-Mohammed T, Koh S, Reaney I, Acquaye A, Schileo G, Mustapha K, et al. Perovskite solar cells: an integrated hybrid lifecycle assessment and review in comparison with other photovoltaic technologies. *Renew Sustain Energy Rev* 2017; 80:1321–44.
- [4] International Energy Agency. Renewable energy market update 2021 outlook for 2021 and 2022; 2021.
- [5] Baetens R, Jelle BP, Thue JV, Tenpierik MJ, Grynning S, Uvsløkk S, et al. Vacuum insulation panels for building applications: a review and beyond. *Energy Build* 2010;42:147–72.
- [6] Franz M, Piringer G. Market development and consequences on end-of-life management of photovoltaic implementation in Europe. *Energy Sustain Soc* 2020; 10:1–21.
- [7] European Commission. Directive (EU) 2018/2001 of the European parliament and of the council of 11 December 2018 on the promotion of the use of energy from renewable sources; 2018.
- [8] Massobrio C, Bouzid A, Boero M, Ori G, Coasne BA. Surface of glassy GeS<sub>2</sub>: a model based on a first-principles approach; 2014.
- [9] Leccisi E, Raugel M, Fthenakis V. The energy and environmental performance of ground-mounted photovoltaic systems—a timely update. *Energies* 2016;9(8):622. <https://doi.org/10.3390/en9080622>.
- [10] Muteri V, Cellura M, Curto D, Franzitta V, Longo S, Mistretta M, et al. Review on life cycle assessment of solar photovoltaic panels. *Energies* 2020;13:252.
- [11] Wong LH, Zakutayev A, Major JD, Hao X, Walsh A, Todorov TK, et al. Emerging inorganic solar cell efficiency tables (Version 1). *J Phys: Energy* 2019;1:032001.
- [12] Vidal-Fuentes P, Placidi M, Sánchez Y, Becerril-Romero I, Andrade-Arvizu J, Jehl Z, et al. Efficient Se-rich Sb<sub>2</sub>Se<sub>3</sub>/CdS planar heterojunction solar cells by sequential processing: control and influence of Se content. *Solar RRL* 2020;4:2000141.
- [13] Lunardi MM, Dias PR, Deng R, Corkish R. Life cycle environmental assessment of different solar photovoltaic technologies. In: Ren J, Kan Z, editors. *Photovoltaic sustainability and management*. AIP Publishing; 2021. p. 1–34. [https://doi.org/10.1063/9780735423152\\_005](https://doi.org/10.1063/9780735423152_005).
- [14] Parsons S, Poyntz-Wright O, Kent A, McManus MC. Green chemistry for stainless steel corrosion resistance: life cycle assessment of citric acid versus nitric acid passivation. *Mater Today Sustain* 2019;3–4:100005.
- [15] Maranghi S, Parisi ML, Basosi R, Sinicropi A. Environmental profile of the manufacturing process of perovskite photovoltaics: harmonization of life cycle assessment studies. *Energies* 2019;12(19):3746. <https://doi.org/10.3390/en12193746>.
- [16] International Organization for Standardization. Environmental management: life cycle assessment; Principles and Framework, ISO; 2006a.
- [17] International Organization for Standardization. Environmental management: life cycle assessment; requirements and guidelines, ISO Geneva, Switzerland; 2006b.
- [18] Collier J, Wu S, Apul D. Life cycle environmental impacts from CZTS (copper zinc tin sulfide) and Zn<sub>3</sub>P<sub>2</sub> (zinc phosphide) thin film PV (photovoltaic) cells. *Energy* 2014;74:314–21.
- [19] Dhimish M, Alrashidi A. Photovoltaic degradation rate affected by different weather conditions: a case study based on PV systems in the UK and Australia. *Electronics* 2020;9(4):650. <https://doi.org/10.3390/electronics9040650>.
- [20] Fthenakis V, Frischknecht R, Raugel M, Kim HC, Alsema E, Held M, et al. Methodology guidelines on life cycle assessment of photovoltaic electricity. IEA PVPS Task 2011;12.
- [21] Wallace SK, Mitzi DB, Walsh A. The steady rise of Kesterite solar cells. *ACS Energy Lett* 2017;2:776–9.

- [22] ZubeI I, Rola K, Kramkowska M. The effect of isopropyl alcohol concentration on the etching process of Si-substrates in KOH solutions. *Sens Actuators, A* 2011;171: 436–45.
- [23] Satoh T, Hashimoto Y, Shimakawa S-I, Hayashi S, Negami T. Cu(In, Ga)Se<sub>2</sub> solar cells on stainless steel substrates covered with insulating layers. *Sol Energy Mater Sol Cells* 2003;75:65–71.
- [24] Noufi R, Zweibel K. High-efficiency CdTe and CIGS thin-film solar cells: highlights and challenges; 2006.
- [25] Nuss P, Eckelman MJ. Life cycle assessment of metals: a scientific synthesis. *PLoS ONE* 2014;9:e101298.
- [26] USGS. Commodity Statistics and Information [Online]; 2021. Available: <https://www.usgs.gov/centers/nmic/commodity-statistics-and-information#Z> [accessed 30/04/2021 2021].
- [27] González díaz g, hernández rojas j, lucía mulas ml, santamaría sánchez-barriga j, sánchez quesada f. Stoichiometry control over a wide composition range of sputtered CuGa<sub>(x)</sub> In<sub>(1-x)</sub> Se<sub>(2)</sub>. *Appl Phys Lett* 1994;64:1239–41.
- [28] Amarakoon S, Vallet C, Curran MA, Haldar P, Metacarpa D, Fobare D, et al. Life cycle assessment of photovoltaic manufacturing consortium (PVMC) copper indium gallium (di)selenide (CIGS) modules. *Int J Life Cycle Assess* 2018;23: 851–66.
- [29] Fernandes LJ, Aroche AF, Schuck A, Lamberty P, Peter CR, Hasenkamp W, et al. Silver nanoparticle conductive inks: synthesis, characterization, and fabrication of inkjet-printed flexible electrodes. *Sci Rep* 2020;10:8878.
- [30] Fields JD, Dabney MS, Bollinger VP, Hest MFAMV. Printed monolithic interconnects for photovoltaic applications. In: 2014 IEEE 40th photovoltaic specialist conference (PVSC), 8–13 June 2014; 2014. p. 0162–0165.
- [31] Dreyer LC, Niemann AL, Hauschild MZ. Comparison of three different LCIA methods: EDIP97, CML2001 and Eco-indicator 99. *Int J Life Cycle Assess* 2003;8: 191–200.
- [32] Frischknecht R, Wyss F, Büsser Knöpfel S, Lützkendorf T, Balouktsi M. Cumulative energy demand in LCA: the energy harvested approach. *Int J Life Cycle Assess* 2015;20:957–69.
- [33] Chomkhamri K, Wolf M-A, Pant R. International reference life cycle data system (ILCD) handbook: review schemes for life cycle assessment. *Towards Life Cycle Sustain Manage* 2011:107–17.
- [34] Jolliet O, Margni M, Charles R, Humbert S, Payet J, Rebitzer G, et al. IMPACT 2002 +: a new life cycle impact assessment methodology. *Int J Life Cycle Assess* 2003;8: 324–30.
- [35] Laurent A, Hauschild MZ. Normalisation. *Life cycle impact assessment*. Springer; 2015.
- [36] Ozturk M, Dincer I. Life cycle assessment of hydrogen-based electricity generation in place of conventional fuels for residential buildings. *Int J Hydrogen Energy* 2020;45:26536–44.
- [37] Giraldo S, Neuschitzer M, Thersleff T, López-Marino S, Sánchez Y, Xie H, et al. Large efficiency improvement in Cu<sub>2</sub>ZnSnSe<sub>4</sub> solar cells by introducing a superficial Ge nanolayer. *Adv Energy Mater* 2015;5:1501070.
- [38] Benhaddou N, Aazou S, Fonoll-Rubio R, Sánchez Y, Giraldo S, Guc M, et al. Uncovering details behind the formation mechanisms of Cu<sub>2</sub>ZnGeSe<sub>4</sub> photovoltaic absorbers. *J Mater Chem C* 2020;8:4003–11.
- [39] European Commission. Critical raw materials resilience: charting a path towards greater security and sustainability. Brussels: European Commission; 2020.
- [40] Alsema E, De Wild-Scholten M, Fthenakis V. Environmental impacts of PV electricity generation—a critical comparison of energy supply options. In: 21st European photovoltaic solar energy conference; 2006. p. 3201–7.
- [41] De Wild-Scholten M. Energierücklaufzeiten für PV-module und systeme energy payback times of PV modules and systems. *Workshop Photovoltaik-Moduletechnik* 2009;27.
- [42] Fthenakis VM, Kim H-C. Energy use and greenhouse gas emissions in the life cycle of thin film CdTe photovoltaics. In: *Proceedings of the symposium G-life cycle analysis, materials research society fall meeting, Boston, MA, USA; 2005*.
- [43] Fthenakis V, Kim H, Held M, Raugei M, Krones J. Update of PV energy payback times and life-cycle greenhouse gas emissions. In: 24th European photovoltaic solar energy conference and exhibition; 2009. p. 21–5.
- [44] Giacchetta G, Leporini M, Marchetti B. Evaluation of the environmental benefits of new high value process for the management of the end of life of thin film photovoltaic modules. *J Cleaner Prod* 2013;51:214–24.
- [45] Held M, Ilg R. Update of environmental indicators and energy payback time of CdTe PV systems in Europe. *Prog Photovoltaics Res Appl* 2011;19:614–26.
- [46] Ito M, Kato K, Komoto K, Kichimi T, Kurokawa K. A comparative study on cost and life-cycle analysis for 100 MW very large-scale PV (VLS-PV) systems in deserts using m-Si, a-Si, CdTe, and CIS modules. *Prog Photovoltaics Res Appl* 2008;16: 17–30.
- [47] Ito M, Komoto K, Kurokawa K. Life-cycle analyses of very-large scale PV systems using six types of PV modules. *Curr Appl Phys* 2010;10:S271–3.
- [48] Li T, Roskilly AP, Wang Y. Life cycle sustainability assessment of grid-connected photovoltaic power generation: a case study of Northeast England. *Appl Energy* 2018;227:465–79.
- [49] Kato K, Hibino T, Komoto K, Ihara S, Yamamoto S, Fujihara H. A life-cycle analysis on thin-film CdS/CdTe PV modules. *Sol Energy Mater Sol Cells* 2001;67:279–87.
- [50] Kim H, Cha K, Fthenakis VM, Sinha P, Hur T. Life cycle assessment of cadmium telluride photovoltaic (CdTe PV) systems. *Sol Energy* 2014;103:78–88.
- [51] Rajput P, Singh YK, Tiwari GN, Sastry OS, Dubey S, Pandey K. Life cycle assessment of the 3.2 kW cadmium telluride (CdTe) photovoltaic system in composite climate of India. *Sol Energy* 2018;159:415–22.
- [52] Raugei M, Bargigli S, Ulgiati S. Life cycle assessment and energy pay-back time of advanced photovoltaic modules: CdTe and CIS compared to poly-Si. *Energy* 2007; 32(8):1310–8.
- [53] Bergesen JD, Heath GA, Gibon T, Suh S. Thin-film photovoltaic power generation offers decreasing greenhouse gas emissions and increasing environmental co-benefits in the long term. *Environ Sci Technol* 2014;48:9834–43.
- [54] Stamford L, Azapagic A. Environmental impacts of copper-indium-gallium-selenide (CIGS) photovoltaics and the elimination of cadmium through atomic layer deposition. *Sci Total Environ* 2019;688:1092–101.
- [55] Van Der Hulst MK, Huijbregts MA, Van Loon N, Theelen M, Kootstra L, Bergesen JD, et al. A systematic approach to assess the environmental impact of emerging technologies; 2020.
- [56] Jungbluth N, Dones R, Frischknecht R. Life cycle assessment of photovoltaics; update of the ecoinvent database. *MRS Online Proceedings Library (OPL)*; 2007. p. 1041.
- [57] Mokhtarimehr M, Forbes I, Pearsall N. Environmental assessment of vacuum and non-vacuum techniques for the fabrication of Cu<sub>2</sub>ZnSnS<sub>4</sub> thin film photovoltaic cells. *Jpn J Appl Phys* 2018;57:08RC14.
- [58] Friedlmeier TM, Jackson P, Bauer A, Hariskos D, Kiowski O, Wuerz R, et al. Improved photocurrent in Cu(In, Ga)Se<sub>2</sub> solar cells: from 20.8% to 21.7% efficiency with CdS buffer and 21.0% Cd-free. *IEEE J Photovoltaics* 2015;5: 1487–91.
- [59] De Wild-Scholten MM. Energy payback time and carbon footprint of commercial photovoltaic systems. *Solar Energy Mater Solar Cells* 2013;119:296–305.