

A systematic approach to assess the environmental impact of emerging technologies

A case study for the GHG footprint of CIGS solar photovoltaic laminate

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Abstract

Estimating the environmental impact of emerging technologies at different stages of development is uncertain but necessary to guide investment, research, and development. Here, we propose a systematic procedure to assess the future impacts of emerging technologies. In the technology development stage (technology readiness level < 9), the recommended experience mechanisms to take into account are (a) process changes, (b) size scaling effects, and (c) process synergies. These developments can be based on previous experience with similar technologies or quantified through regression or engineering dimension calculations. In the industrial development phase, (d) industrial learning, based on experience curves or roadmaps, and (e) external developments should be included. External developments, such as changes in the electricity mix can be included with information from integrated assessment models. We show the applicability of our approach with the greenhouse gas (GHG) footprint evaluation for the production of copper indium gallium (di)selenide (CIGS) photovoltaic laminate. We found that the GHG footprint per kilowatt peak of produced CIGS laminate is expected to decrease by 83% going from pilot to mature industrial scale production with the largest decrease being due to expected process changes. The feasibility of applying our approach in practice would greatly benefit from the development of a database containing information on size scaling and experience rates for a wide variety of materials, products, and technologies.

KEYWORDS

environmental experience curve, ex ante, industrial ecology, life cycle assessment (LCA), prospective, technological innovation

1 | INTRODUCTION

Emerging technologies are expected to have a profound contribution to sustainable development, although their utilization can also create a complex web of unforeseen negative environmental consequences (United Nations, 2018). Life cycle assessment (LCA) is therefore increasingly applied to predict future environmental impacts of emerging technologies in order to obtain insights in pathways toward minimizing these impacts (Bergeron et al., 2020). The insights obtained from such LCAs are particularly valuable at the early stage of technology development, because substantial redesign of product and processes can still be implemented with relative ease and at lower costs.

The use of LCA in an early stage of technological development has been studied since the 1990s (e.g., Azapagic, 1999) and has since continued to develop under diverse names. These include anticipatory (Collier, Connelly, Polmateer, & Lambert, 2017; Wender et al., 2014), early stage

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(Hetherington, Borrión, Griffiths, & McManus, 2014), emerging (Barberio, Scalbi, Buttol, Masoni, & Righi, 2014; Tsang, Bates, Madison, & Linkov, 2014), ex ante (Fazeni, Lindorfer, & Prammer, 2014; Villares, Işıldar, Beltran, & Guinée, 2016; Villares, Işıldar, van der Giesen, & Guinée, 2017), prospective (Arvidsson et al., 2017; Miller & Keoleian, 2015; Simon, Bachtin, Kiliç, Amor, & Weil, 2016), and screening LCA (Hung, Ellingsen, & Majeau-Bettez, 2020). As aptly summarized by Bergerson et al. (2020), this “diversity of terms mirrors the wide range of available methods and disparate language employed across the LCA community.”

Several recent publications have listed the observed approaches in LCA with a definition or description (Buyle, Audenaert, Billen, Boonen, & Van Passel, 2019; Cucurachi, van der Giesen, & Guinée, 2018; Guinée, Cucurachi, Henriksson, & Heijungs, 2018; van der Giesen, Cucurachi, Guinée, Kramer, & Tukker, 2020). Assessments of emerging technologies, studied at an early phase, are typically labeled either “prospective” or “ex ante” LCA. Indeed, van der Giesen et al. (2020) regard these umbrella terms for the same exercise. However, they argue that the term ex ante indicates assessment before market introduction of a technology, whereas prospective LCA can also be performed on established technologies to estimate future environmental impacts. In this paper we use the term prospective LCA and adopt the definition from Arvidsson et al. (2017) that “an LCA is prospective when the (emerging) technology studied is in an early phase of development (e.g., small-scale production), but the technology is modeled at a future, more-developed phase (e.g., large-scale production).” As pointed out by Buyle et al. (2019), the term “emerging technology” has seen similar ambiguity. In this paper we apply the same definition as they adopted, which defines emerging technologies as “technologies that are still under development and are not ready yet to enter the market.”

Environmental impacts identified at an early stage of technology development are not necessarily representative for the technology in its final form. A reduction in environmental impacts per unit output may be observed when studying the maturation of an emerging technology as it goes from an early phase to a more-developed phase. A technology is considered mature when it has reached a state of pervasive market diffusion and has well-known characteristics (Grübler, Nakićenović, & Victor, 1999). The reduction in environmental impact due to technological maturation is mainly attributed to two distinct processes: scaling and learning. Size scaling factors relate environmental effects to size or capacity of products or technologies (Caduff, Huijbregts, Althaus, & Hendriks, 2011; Caduff, Huijbregts, Althaus, Koehler, & Hellweg, 2012; Caduff, Huijbregts, Koehler, Althaus, & Hellweg, 2014), while learning and experience rates relate environmental effects to cumulative production as a measure of experience (Caduff et al., 2012). Gavankar, Suh, and Keller (2015) showed, for instance, that impacts per unit output decrease as technologies become more developed. Besides the use of experience rates, Simon et al. (2016) and Piccinno, Hirschier, Seeger, and Som (2016) developed approaches to estimate industrial scale performance through extrapolation from available lab data. Arvidsson et al. (2017) further highlighted the importance of using scenarios for possible future developments, which should be used to prevent temporal mismatches between the technological development rates of the foreground and background systems. For instance, when studying the future environmental impact of a production process in 2030 (foreground system), one should also use a representative electricity mix that matches with projections for 2030 (background system).

Several recent studies have identified existing challenges in modeling emerging technologies at a future point in time and list available methods, concepts, and recommendations to provide guidance to LCA practitioners that conduct prospective LCAs of these emerging technologies. Four main challenges were identified by Hetherington et al. (2014), which are comparability between technologies, scaling issues, data availability, and uncertainty. These challenges are also listed in reviews on LCA of emerging technologies by Moni, Mahmud, High, and Carbajales-Dale (2020) and Thonemann, Schulte, and Maga (2020). Alternatively, Bergerson et al. (2020) categorize the challenges in prospective LCA for emerging technologies on the basis of technology characteristics and market context, thereby distinguishing between technologies or markets that are either emerging or mature. Another approach is presented by van der Giesen et al. (2020), who evaluate the challenges in prospective LCA of emerging technologies by following the four phases of LCA discerned in the ISO 14040 standard. All acknowledge the main drivers of technology maturation—scaling and learning—as relevant mechanisms to take into account in prospective LCA of emerging technologies. The work of Buyle et al. (2019) deserves special attention, for they provide an extensive overview of techniques to upscale technologies and model continuous improvement of mature technologies. While all of these studies provide valuable contributions to organize the relevant steps and provide practical recommendations for prospective LCA, an explicit, overarching protocol for performing a prospective LCA, including a demonstration of its application, is missing.

Here, we propose a systematic approach to evaluate the environmental impact of emerging technologies. Relevant steps of technological development were identified through an extensive literature research of prospective LCAs and were ordered according to the development stage of a technology from early stage to mature. Our approach aims to facilitate prospective LCA practitioners and enable a representative estimation of future environmental impacts for emerging technologies, allowing for a fair comparison with mature, established technologies. This study provides an organized procedure for conducting prospective LCA by categorizing and arranging relevant steps and includes a case study in which the application of this approach is demonstrated.

Below, the steps and mechanisms of our systematic approach are described in more detail, and subsequently applied in practice to the thin film photovoltaic (PV) technology known as copper indium gallium (di)selenide (CIGS). This technology was selected because of the on-going research into design optimization, the known mechanisms for technological developments and the in-house availability of data.

2 | SYSTEMATIC ENVIRONMENTAL EVALUATION OF EMERGING TECHNOLOGIES

A technology's observed maturation can be attributed to different experience mechanisms and developments. All of these were identified through an extensive literature review, which is described in the next sections. We propose a systematic approach for use in prospective LCA that (a) addresses all these mechanisms and developments and (b) examines these in an explicit order. Our approach is defined in three different phases, in which the different steps are structured in a consecutive order. A graphical representation is displayed in Figure 1 and its description is summarized in Table 1.

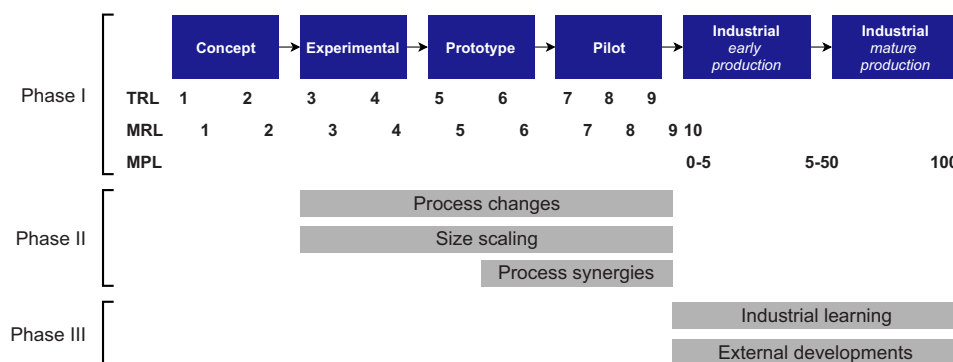


FIGURE 1 Levels and mechanism in technology development. TRL, technology readiness level; MRL, manufacturing readiness level; MPL, market penetration level. Grey boxes indicate experience mechanisms and developments, length of the boxes indicates at which development stages these mechanism and developments mainly occur. Terminology of the stages (blue square boxes) is taken from Villares et al. (2017)

TABLE 1 Descriptions and modeling methods for the different steps in the systematic approach

Phase: Step	Description	Modeling method
Phase I: Definition of the development stage	Identify the current level of technological readiness or maturity in order to establish which development steps are still to be implemented in the timeframe under consideration	NA
Phase II: Process changes	Changes to processing methods due to the availability of or necessity for other equipment and materials. These changes typically improve product performance and/or allow for cheaper and safer production at larger scales	Deduction from existing industrial processes through an analysis of functions, dimensions, and similarities
Phase II: Size scaling	Changes of the physical dimensions of the product (product scaling) and/or the increase in equipment dimensions to accommodate larger products, larger production volumes, or both (equipment scaling)	Engineering geometry calculations or log-linear regression of scaling curves that relate size parameters to key properties of the technology's environmental impact
Phase II: Process synergies	Minimization or valorization of final waste streams through the application of recovery and recycling options for materials and energy. Potential co- and/or by-products are dealt with through allocation, system expansion, or exclusion. The analysis of process synergies is typically not applied before TRL 5	Deduction from plant flow charts of existing industrial production processes
Phase III: Industrial learning	All learning and experience mechanisms in industrial scale production, (e.g., learning-by-doing, learning-by-searching, production scaling, production line synergies). These mechanisms are typically difficult to disentangle and might therefore also be studied collectively and quantified as a single development factor for a company or industry	Log-linear regression of experience curves that relate cumulative production to the environmental impact of a produced unit
Phase III: External developments	Future developments in external systems that influence the production of the studied technology or its upstream or downstream processes	Combining LCA with integrated assessment models (IAMs)

NA, not applicable.

Phase I defines the current development stage for the studied technology in terms of technology readiness levels (TRLs), manufacturing readiness levels (MRLs), or market penetration levels (MPLs). Phase I belongs to the goal and scope definition stage of conventional LCA and is done to determine which developments are likely to still occur and are therefore relevant to examine. In phase II, three development mechanisms toward technology and manufacturing readiness are examined consecutively, which are “process changes,” “size scaling,” and “process synergies.” Industrial production and a product market are not yet considered for this phase. The grey bars in Figure 1 illustrate the ranges where these mechanisms might occur along the overall development process. The development of a technology is typically an iterative process in which each of the three mechanisms can repeatedly occur anywhere in their described ranges, either consecutively or simultaneously. However, for the analysis of the overall development process, it is recommended to study these mechanisms in the proposed order. This is because in the life cycle inventory (LCI) stage, one typically starts with constructing a process tree, then quantifies all the processes in this tree, and finally allocates any quantities between output flows, if necessary. We argue that the composition of the process tree is typically influenced by process changes, while size scaling generally influences the quantities of the processes, and process synergies mostly influence allocation between product systems. In phase III, two industrial developments are identified, which are “industrial learning” and “external developments.” No distinct order is proposed for studying these mechanisms. In the following sections, all three phases and the allotted mechanisms and developments are described in more detail.

2.1 | Phase I: Definition of the development stage

Stages in technology development can be characterized according to TRLs, MRLs, MPLs, and production scale. The TRL is a measure of functional readiness of the product, whereas the MRL is a measure of readiness for production. The descriptions of the TRLs/MRLs are condensed by Gavankar et al. (2015) and can be grouped into conceptual development (TRL/MRL 1–4), technology development (TRL/MRL 5 and 6), engineering development (TRL/MRL 7), small-scale production (TRL/MRL 8 and 9), and mass production (MRL 10). For a more comprehensive description of the distinct levels and the differences in TRL and MRL, we refer the reader to the work of Gavankar et al. (2015) and Moni et al. (2020). Beyond a product's functional and manufacturing readiness, its market share can be described by increased production numbers and scale. The MPLs are taken from Gröbler et al. (1999): invention and innovation (0% market penetration), niche market commercialization (0–5% market penetration), pervasive diffusion (5–50% market penetration), and saturation (up to 100% market penetration for a monopoly). Once the current development stage is identified, the relevant experience mechanisms and developments of phases II and III can be studied more closely.

2.2 | Phase II: Assessment of developments toward technology and manufacturing readiness

2.2.1 | Process changes

In the development stages from “experimental lab” via “prototype” to “pilot,” the production process itself may completely change. This could be due to the availability of or necessity for other equipment and materials. In this phase, process improvements are referred to as learning by research (e.g., Rivera-Tinoco, Schoots, & van der Zwaan, 2012). Changes resulting in cheaper and safer production should also be taken into account, since these criteria are considered the main driving forces for process optimization toward product commercialization. Additionally, process changes that improve product performance should be included (e.g., the increased range for electric vehicles). Process changes can be modeled in the LCI by altering the material processes that make up the process tree.

For products that are under development, process changes can be deduced from existing industrial processes with similarity analysis (Simon et al., 2016). This procedure includes an analysis of functions and similarities, respectively. In the analysis of functions, the function of a lab process step is defined and an industrial scale process with the same function is identified (e.g., mixing in Erlenmeyer or in stainless steel tank). This results in an industrial scale process chain built of known processes. In the analysis of similarities, the characteristics of the large-scale process are defined, such as energy requirements for equipment. Finally, this information is combined to estimate the inputs and outputs of the industrial process. These similarity analyses allow for extrapolation of process changes through expert predictions of expected developments, industry communications of proposed development strategies (whitepapers), and industry instructions for concrete development targets with deadlines (roadmaps). It is important to ensure that modeled process changes comply with existing regulations for technologies, such as product quality and safety standards.

2.2.2 | Size scaling

Scaling of product and equipment, which are forms of size scaling, can play a role in the development toward technological readiness. Product scaling is the change in the physical dimensions of a product and is most prominent when going from experimental to pilot scale. While product scaling often results in increased product dimensions, in some cases a decrease might be pursued (e.g., for portable electronic devices). Equipment scaling has also been termed “apparatus scale up to extend processing capacity” by Shibasaki, Fischer, and Barthel (2007). Its influence seems particularly prominent when going from pilot to industrial scale. For instance, De Marco, Iannone, Miranda, and Riemma (2018) found larger

relative changes in environmental impacts for 13 out of 15 impact categories when going from pilot to industrial than when going from bench to pilot scale production equipment.

Regressions are used to relate key properties to the size of the technology or production equipment, resulting in size scaling curves. Several studies derived size scaling curves, for instance, for energy conversion equipment (Caduff et al., 2011), heat production (Caduff et al., 2014), chemical production (Piccinno, Hischer, Seeger, & Som, 2018), milk homogenization (Valsasina et al., 2017), and bioleaching (Villares et al., 2017). It is convention in scaling studies to perform linear regression on log transformed data, with size scaling relations generally taking the form of Equation (1).

$$\log(EI) = \log(a) + b \cdot \log(S) \quad (1)$$

Where EI is the environmental impact per functional unit of the scaled technology, $\log(a)$ is the intercept of linear regression, b is the size scaling factor (unitless), and S represents the scale of the technology. For the example of a heat pump of a certain size (Caduff et al., 2014), EI equals the impact per MJ heat produced (e.g., kg CO₂ equiv./MJ) and S is the power output of the heat pump in kW (e.g., 100 kW). Equation (1) can also be applied to scale elementary material or energy flows in the LCI of the scaled technology.

Scaling factors can also be derived from engineering calculations based on geometry (Caduff et al., 2012; Piccinno et al., 2016). For instance, Piccinno et al. (2016) derived that the energy required for stirring in a chemical reactor was inversely proportional to the diameter of the reactor, which can be linked to the reactor volume through geometry.

2.2.3 | Process synergies

Once a production process starts to take shape at around TRL 5 or higher, the minimization of waste streams becomes increasingly relevant. Production line synergies occurring at the plant level, such as recovery and reuse of heat, can reduce total energy demand (Piccinno et al., 2016). These types of process synergies might already be tested and/or implemented at a prototype or pilot stage. Other processes, such as recovery of solvents, generation of by- and co-products, and treatment of waste, should also be considered. Piccinno et al. (2016) recommend the use of scenario analysis if treatment options are still unknown (e.g., solvent recovery or discharge). Changes in the LCI due to process synergies can be accommodated through allocation, system expansion, or exclusion.

2.3 | Phase III: Assessment of developments for industrially produced technologies

2.3.1 | Industrial learning

On the scale of industrial production, learning by doing is expected to be the dominant mechanism for reducing environmental impacts (as shown by Caduff et al., 2012). Additionally, size scaling and process synergies as defined and studied in phase II can also occur on the industrial level. However, contributions of different learning mechanisms are often difficult to disentangle at the industrial scale and might therefore also be studied collectively and quantified as a single experience curve for a company or industry.

To this end, learning and experience curves can be used, which are widely applied in, for example, economics to estimate future cost developments (e.g., energy models (Berglund & Söderholm, 2006); metal tube hydroforming (Nadeau, Kar, Roth, & Kirchain, 2010); airplanes (Wright, 1936)). Learning curves describe the empirical correlation between the reduction in labor time or costs per produced unit and the cumulative production quantity. Wright's model for learning curves is the most commonly used and consists of a log-linear curve varying with cumulative production volume (Nadeau et al., 2010). Experience curves are similar to learning curves, but cover a broader scope. Where learning curves are limited to describe cost reduction through learning-by-doing, experience curves can also include other learning mechanisms, such as economies of scale. The concept of experience curves has been applied to a limited extent in environmental science to describe a reduction of environmental impact per produced unit as a function of cumulative production. Caduff et al. (2012) showed how to derive environmental experience curves for wind turbines, based on previously performed LCA studies, using Equation (2).

$$\log(EI_{cum}) = \log(EI_0) + z_e \cdot \log(Cum) \quad (2)$$

Where EI_{cum} is the environmental impact for the last produced unit (e.g., kg CO₂ equiv./MJ), EI_0 is the environmental impact of the first unit produced (e.g., kg CO₂ equiv./MJ), z_e is the environmental experience factor (unitless), and Cum is the cumulative production count (e.g., total number of units produced). Equation (2) can also be applied to elementary material or energy flows in order to compose a supply-chain learning curve for a technology, as demonstrated by Bergesen and Suh (2016). The environmental experience factor (z_e) can be used to derive the environmental progress rate (pr_e) and environmental learning rate (lr_e) with Equation (3).

$$pr_e = 2^{z_e} = 1 - lr_e \quad (3)$$

Both the progress rate and environmental learning rate are typically expressed as a percentage, with, for example, a learning rate of 20% (progress rate of 80%) indicating that for every doubling in cumulative production, the environmental impacts per produced unit decreases by 20%. The environmental learning rate thus provides a way to quantify the continued environmental impact reduction of a technology taken into mass production.

2.3.2 | External developments

While developing a new technology, changes could occur in other parts of the economy as well. On the one hand, these could be the implementation of alternative (existing or emerging) technologies. On the other hand, changes may occur in background processes, both upstream or downstream, such as electricity and heat production (upstream), waste treatment (downstream), or transport (upstream and downstream). While these external developments typically originate from interactions in the technosphere, developments in the biosphere such as global warming or ozone layer depletion can result in legislation that could also be a driving force for technological development. Arvidsson et al. (2017) defined the term of prospective LCA as being one conducted at time zero, but aiming to describe the situation at a future moment in time. As such, they point out that not only changes related to the technology itself should be accounted for, but also a number of other changes in external factors. These external developments take on two different forms.

First of all, the selection of a reference technology should be broader than the current most used alternative, as that might not be the most likely alternative in the future. Other technologies might be under development that could become alternatives to the one under investigation. Arvidsson et al. (2017) cite the example of battery choices in electric vehicles: early assessments would have chosen lead acid batteries as a reference, but today they would not be considered a good proxy for electric vehicles, since these currently use lithium ion batteries.

Second, background inventory data should match in time, for example, if an emerging technology is assessed for a future moment in time, the supply chain should take into account the future electricity mix. Experience in external (i.e., supply chain) processes can also be taken into account (Bergesen & Suh, 2016). In the analysis of wind electricity for the UK, Wiedmann et al. (2011) included changes in the background electricity mix. They proposed integrated hybrid LCA as a way to take into account the effects of emerging energy generation technologies on these electricity mixes and derived impacts. Cox, Mutel, Bauer, Beltran, and van Vuuren (2018) incorporated results from an integrated assessment model (IAM) into LCI data to reflect future changes in the electricity provision.

3 | CASE STUDY: SOLAR PV APPLICATION AND EVALUATION

3.1 | Case description

An LCA case study from the PV sector is conducted to demonstrate the application of the proposed systematic approach. The case study relates to the production of the thin film PV technology CIGS. The goal of the case study was to compare the greenhouse gas (GHG) footprint of the pilot scale production of rigid CIGS laminate with the future industrial scale production of flexible CIGS laminate. A cradle-to-gate analysis was conducted, excluding the use phase and end-of-life treatment of the PV laminate. The functional unit for this case study was the production of 1 kilowatt peak (kW_p) of CIGS laminate, which is a subset of the PV panel that contains substrate, absorber and conducting layers, and encapsulant. Dividing the electricity generating capacity of 1 kW_p by the photovoltaic efficiency of the laminate yields the required square meter area of laminate. The assessment was performed with software package SimaPro version 8.5.2.0. (SimaPro, 2018) with inventory database ecoinvent 3.4 (Ecoinvent Centre, 2017; Wernet et al., 2016), system model "allocation, cut-off by classification." Following the ReCiPe 2016 method (Huijbregts et al., 2017), Global Warming Potentials from IPCC (2013) for a 100 year time horizon and including climate feedbacks were used to quantify the GHG footprint, as an illustration of one of the relevant environmental impacts for PV panels. A more comprehensive definition of the goal and scope for the case study is included in Section 1 of Supporting Information S1 and a graphical representation of the product system is depicted in Figure 2.

The pilot scale production process was modeled after a general research set-up at Solliance Thin Film Solar Research in the Netherlands representing the situation in 2014. The pilot scale CIGS laminate had a photovoltaic efficiency of 15% under standard test conditions and was manufactured by depositing the required layers on a $30 \times 30 \text{ cm}^2$ rigid substrate in a bottom-up approach. The architecture of this laminate and the flow of electrons through it is displayed in Figure 3a. Information on required production equipment was collected from CostInsight, which is a cost model developed by TNO/Solliance for internal use to estimate future production costs of thin film applications. The pilot production process is described in more detail in Table 2 and in Section 2 of Supporting Information S1 and an LCI is provided in Table S2–12 of Supporting Information S2.

We modeled the steps from the pilot production process to future industrial production in the year 2030, which is the time horizon for the in-house available roadmap. The modeled developments are described in Table 3 and the resulting changes in the architecture of the laminate are displayed in Figure 3b. The developments toward technology and manufacturing readiness (phase II) were formulated by combining a selection of targets and forecasts for CIGS production optimization described in a roadmap of Solliance (Kuypers, Veenstra, & Schermer, 2018). It is projected that these phase II development targets are reached in 2022. From there on, the steps of phase III are used to model the developments for the

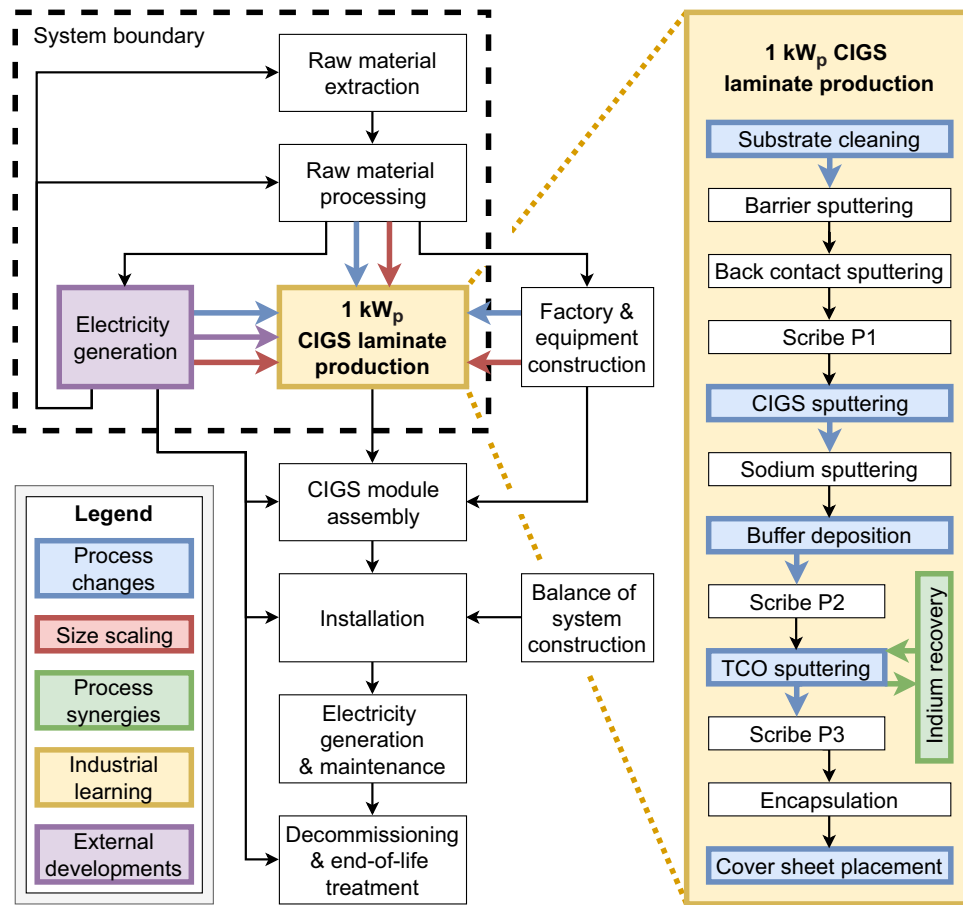


FIGURE 2 Product system with system boundary for the life cycle assessment (LCA) of the production process of copper, indium, gallium, (di)selenide (CIGS) laminate described in the case study. Colored boxes and arrows indicate processes and product flows, respectively, which are affected by developments described in the development scenario. Waste streams and waste treatment are not displayed for simplicity. Transportation is not taken into account, except for the ecoinvent processes in which transportation is defined by default. TCO, transparent conductive oxide

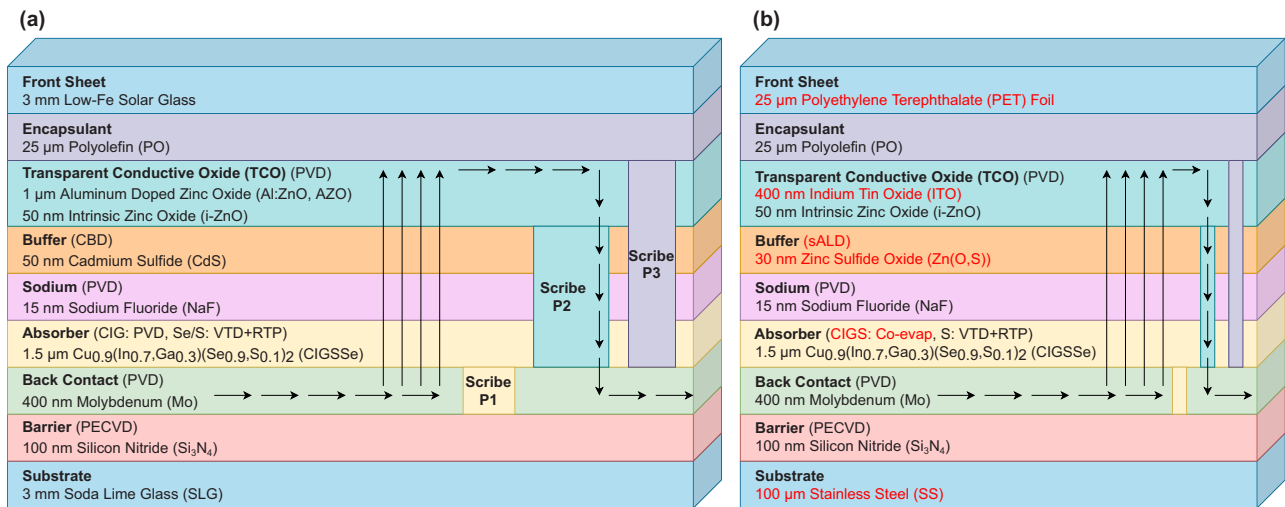


FIGURE 3 Architecture of the CIGS laminate with monolithic interconnection (a) before and (b) after process changes are implemented. These changes are (1) from sheet-to-sheet to roll-to-roll processing, changing the substrate and front sheet material and processing equipment; (2) different buffer material and processing method; (3) different TCO. The changes relative to the pilot production process are marked in red. Black arrows indicate the flow of charge. Processing method abbreviations in parentheses are explained in Table 2. Additional abbreviations are: spatial atomic layer deposition (sALD) and co-evaporation (co-evap)

TABLE 2 Detailed description of the layers in the pilot produced CIGS laminate

Layer: Processing method(s) (abbreviation)	Material (abbreviation)—layer thickness: function
Substrate: NA	Soda lime glass (SLG) —3 mm: Support for absorber and conducting layers
Barrier: Plasma-enhanced chemical vapor deposition (PECVD)	Silicon nitride (Si_3N_4) —100 nm: Eliminates migration of various elements from SLG into the CIGS _{Se} absorber layer
Back contact: Physical vapor deposition (PVD)	Molybdenum (Mo) —400 nm: Conducts charges that are created in the absorber layer and reflects photons back into the absorber layer to increase the overall absorbance
Absorber: Physical vapor deposition (PVD), vapor transport deposition (VTD), and rapid thermal processing (RTP)	Copper, indium, gallium, sulfur, selenium (CIGS_{Se}) —1.5 μm : Absorbs the photons from sunlight and turns their energy into electrons and positively charged holes
Sodium: Physical vapor deposition (PVD)	Sodium fluoride (NaF) —15 nm: Improves the photon absorption process
Buffer: Chemical bath deposition (CBD)	Cadmium sulfide (CdS) —50 nm: Material that is needed in combination with the CIGS _{Se} to create the current
Transparent conductive oxide (TCO): Physical Vapor Deposition (PVD)	Intrinsic zinc oxide (i-ZnO) —50 nm and aluminum-doped zinc oxide (AZO) —1 μm : Transparent electrode that conducts the electrons, created in the absorber layer
Scribe P1, P2, P3: Laser ablation	NA (NA) —NA: Monolithic module interconnection that enables conduction of charge without using electrode grids
Encapsulant: NA	Polyolefin (PO) —25 μm : Encapsulates the absorber and conducting layers to protect them from the elements
Front sheet: NA	Low-iron solar glass —3 mm: Transparent cover material which absorbs as little light as possible

NA, not applicable.

industrially produced CIGS until 2030. The modeled changes are described below, while a more detailed description is given in Sections 3 and 4 of Supporting Information S1.

3.2 | Phase I: Definition of the development stage

To accurately report TRLs for PV technologies, Baliozian et al. (2016) proposed the use of PV-specific definitions as introduced by Fraunhofer ISE. Based on their definitions and categorization by Kato (2016), three development stages for PV cells can broadly be distinguished: TRL 1–4, in which novel concepts are developed and studied in the lab: examples are small solar cells (they are often as small as 0.5 cm²), but also for instance the optimization of interconnection technologies or barrier layers. In the next development stage (TRL 5–7), the concepts are brought to (mini)module development. The final stage is development on an industrial scale (TRL 8–9) with areas of around 120 × 120 cm². While CIGS is a proven technology in production at TRL 9, research into improvement of both the technology and its manufacturing process is still on-going. These improvements go beyond just incremental changes of the technology, but rather constitute emerging iterations of an existing technology. We therefore study an emerging CIGS configuration for which in-house data are available at the prototype stage. The production process for this prototype was demonstrated as a pilot process in an environment suitable for production, which is classified as TRL 5 (Baliozian et al., 2016). To this baseline case we apply our approach for prospective LCA to model the laminate production at TRL 9, MRL 10, and an MPL > 0%.

3.3 | Phase II: Assessment of developments toward technology and manufacturing readiness

A detailed description of the application of phase II is given in Section 3 of Supplementary Information S1. An LCI is provided in Table S2–21 of Supporting Information S2 for the production process after implementing each step of phase II.

3.3.1 | Phase II: Process changes

The selection of the most likely process changes is complicated due to the multitude of processes that are currently used, both in laboratories and in industry. An overview of process steps for commercial companies is provided by Feurer et al. (2016). This reference shows that it is impossible to designate one “scenario” as the relevant “upscaled” scenario. However, it is possible to select some trends from a longer list than provided by Feurer et al. In this case, targets and forecasts of three process changes toward cheaper and safer production of CIGS laminate were taken from the Solliance roadmap (Kuypers et al., 2018). One process change is the shift from sheet-to-sheet (S2S) processing of rigid laminate to roll-to-roll (R2R) processing of flexible laminate. As a result, the glass substrate and front sheet were replaced with a stainless steel substrate and PET-foil front sheet, while S2S processing equipment is replaced with R2R equipment, changing the auxiliaries consumptions of electricity, cooling water and gasses in the production process. For thin film technologies, the shift to R2R is a common trend which reduces production costs. A second change

TABLE 3 Modeled developments for the case study using the proposed systematic approach

Phase: Step	Modeled changes	Pilot scale process (2014)	Industrial process (2030)
Phase I: Definition of the development stage	Technological development	TRL 5, MRL5, MPL 0%	TRL 9, MRL 10, MPL 6%
Phase II: Process changes	<ul style="list-style-type: none"> • Cheaper production • Safer production • Improved performance: Increased lifetime 	<ul style="list-style-type: none"> • Discontinuous rigid sheet-to-sheet (S2S) processing Substrate: 3 mm soda lime glass (SLG); Front sheet: 3 mm low-iron solar glass • Buffer layer with cadmium Buffer: 50 nm CdS • Moisture sensitive TCO TCO: 50 nm i-ZnO and 1 μm Al:ZnO 	<ul style="list-style-type: none"> • Continuous flexible roll-to-roll (R2R) processing Substrate: 100 μm stainless steel (SS); Front sheet: 25 μm PET foil • Cadmium-free buffer layer Buffer: 30 nm Zn(O,S) • Moisture resilient TCO TCO: 50 nm i-ZnO and 400 nm ITO
Phase II: Size scaling	<ul style="list-style-type: none"> • Product scaling • Equipment scaling 	<ul style="list-style-type: none"> • 30 \times 30 cm² laminate • Conveyor width 30 cm 	<ul style="list-style-type: none"> • 90 \times 120 cm² laminate • Conveyor width 120 cm
Phase II: Process synergies	Reduction of final waste streams	Hazardous waste treatment of spent ITO target	Recovery, processing, and reuse of indium from spent ITO targets
Phase III: Industrial learning	General improvements in foreground processes of industrial production as a result of increased production experience	NA	<ul style="list-style-type: none"> • Environmental experience factor: -0.19. • Estimated cumulative CIGS production in 2030: 192,720 MW
Phase III: External developments	Decarbonization of the electricity sector	Known Dutch electricity grid mix for 2014	Estimated Dutch electricity grid mix for 2030 including more technologies with low GHG intensity

NA, not applicable.

was the replacement of the cadmium sulfide (CdS) buffer, containing the toxic element cadmium, to a less toxic, and therefore safer, buffer material consisting of zinc sulfide oxide (Zn(O,S)). The third change was the replacement of the transparent conductive oxide (TCO) made of water sensitive zinc oxides (i-ZnO/AZO) with a TCO made of indium tin oxide (ITO) on i-ZnO, which is less moisture sensitive (Coyle et al., 2013). This increases the lifetime of the laminate, thereby improving the performance of the product as increased lifetime decreases the cost per kWh generated. It is not yet clear which interconnection approach will dominate production of flexible modules in the future. This scenario assumed that the monolithic interconnection approach (consisting of scribes P1, P2, and P3) is conserved, while flexible modules are nowadays often made using a different interconnection method that utilizes a grid of conducting metal on top of the laminate. The architecture of the CIGS laminate after the process changes is displayed in Figure 3b.

3.3.2 | Phase II: Size scaling

Product scaling was modeled as going from a prototype 30 \times 30 cm² to an industrial 90 \times 120 cm² panel size, which is a typical size for panels produced by Solar Frontier, the largest producer of CIGS panels (Solar Frontier, 2016). Consequently, the required industrial equipment is increased with equipment scaling to accommodate the larger product. This larger equipment required more energy, cooling water and gases to operate, but also had a higher output of CIGS laminate. A doubling of substrate width results in a doubling of laminate output, when the conveyor speed is kept constant. However, the doubling in substrate width does not necessarily imply that the production equipment consumes twice as many auxiliaries. Rather, an exponential size scaling ratio is often observed for auxiliary consumption compared to size increase. For the case study, an exponential factor R was applied to the ratio of the large-scale to small-scale substrate width to derive scaled-up consumptions with Equation (4).

$$\frac{C_{2,i}}{C_{1,i}} = \left(\frac{w_2}{w_1} \right)^R \quad (4)$$

where w_1 is the pilot substrate width of the equipment, w_2 the scaled-up substrate width, both having a unit of length (e.g., meter) and C_1 and C_2 are the respective consumption of auxiliaries (index i) of the pilot (1) and upscaled (2) processes, both having a corresponding unit (e.g., kWh for electricity or m³ for water or gas consumptions). The exponential factor R is unitless and for cost scale-up of process equipment it was found to range from as low as 0.1 to as high as 2.6, with an average value of 0.68 as determined from 75 kinds of equipment (Remer & Chai, 1993). Since the exact value for the equipment size scaling cannot be empirically determined for the case study, it was assumed that the average value

of R for cost scale-up of process equipment could also be applied to scaling of auxiliaries consumption and this average value of R was rounded to 0.7.

3.3.3 | Phase II: Process synergies

An example of minimizing a waste stream through recovery and recycling was used to model a process synergy. For this example, the ITO waste stream was minimized by recovering indium from the spent ITO target. Such a target is typically not fully consumed in the sputtering process and the remains contain high concentrations of valuable and scarce indium. The spent ITO target can easily be retrieved for subsequent recovery of this indium. The system was expanded to include material and energy consumptions for this recovery process, which were taken from a study by Gu, Fu, Dodbiba, Fujita, and Fang (2017) on separation and recovery of indium and tin from ITO targets. In the process, thionyl chloride is consumed and hydrochloric acid and sulfur dioxide are formed. The hydrochloric acid can be reused in the process, while the sulfur dioxide can be sold. It is assumed that the recovered indium is sold back for reuse at 25% of the original price (Woodhouse et al., 2013), which was modeled by multiplying the recovered mass of indium by 0.25. Final losses were treated as hazardous waste.

3.4 | Phase III: Assessment of developments for industrially produced CIGS

A detailed description of the application of phase III is given in Section 4 of Supplementary Information S1.

3.4.1 | Phase III: Industrial learning

The influence of industrial learning on reducing the GHG footprint of CIGS production was estimated with an environmental experience curve. Bergesen and Suh (2016) derived an environmental experience curve for cadmium telluride (CdTe) thin film PV modules, which have the same technological characteristics as CIGS. They found an environmental learning rate (lr_e) of 12.5% when excluding learning in upstream processes. It follows from Equation (3) that the environmental experience factor (z_e) for CdTe is -0.19 . The GHG footprint of CIGS production in 2030 (El_{cum}) was estimated with Equation (2) by applying the same z_e and using estimates of cumulative CIGS production (Cum) for 2022 (end of phase II) and 2030. Historic data (2007–2017) on CIGS production (Fraunhofer ISE, 2019) were extrapolated to 2030 using future development estimates for the global cumulative installed capacity of PV (Kost, Shammugam, Jülch, Nguyen, & Schlegel, 2018).

3.4.2 | Phase III: External developments

Future developments of the electricity grid mix will most likely result in a lowering of the average GHG footprint per kW_p of laminate produced, independent of progress in the production technology itself. Predictions on the GHG intensity and composition of technologies for the electricity markets of 2030 were taken from the IAM E3ME-FTT-GENIE (Mercure et al., 2018), assuming a scenario consistent with policies aimed at a maximum global warming of $2^\circ C$. The electricity production mix in ecoinvent for the Netherlands was adjusted for these composition changes and subsequently applied in the modeled foreground system. The LCI for the adapted electricity production mix of the Netherlands is included in Table S2–27 of Supporting Information S2.

3.5 | GHG footprint results

The GHG footprint for the production of the rigid $30 \times 30 \text{ cm}^2$ prototype CIGS laminate for the reference year 2014 is $230 \text{ kg CO}_2 \text{ equiv./kW}_p$. In Figure 4, a decomposition of this GHG footprint is provided for the different layers and select contributors. The use of electricity and glass contributed the most to the overall GHG footprint.

The GHG footprint per kW_p of CIGS laminate produced in 2030 was estimated to be $40 \text{ kg CO}_2 \text{ equiv./kW}_p$, which is an expected lowering in GHG footprint of 83% from pilot to industrial scale production of CIGS. Figure 5 displays the reductions in GHG footprint per kW_p of CIGS laminate produced for each of the experience mechanisms and developments described in phases II and III of the proposed systematic approach. Process changes were found to cause the largest decrease in overall GHG footprint, mainly due to the replacement of the glass substrate and cover sheet. Process changes and size scaling resulted in the utilization of different equipment with lower power demands, thereby reducing electricity consumptions. Process synergies reduced consumptions of indium, which had a marginal contribution to the overall GHG footprint. For industrial learning, separate contributions of underlying mechanisms such as learning-by-doing and learning-by-searching could not be distinguished since a single experience rate was applied. External developments decreased the GHG intensity of the consumed electricity in the production process, which resulted in a small decrease in total GHG footprint. This decrease was small because the process changes and size scaling had already decreased electricity consumption in the production process.

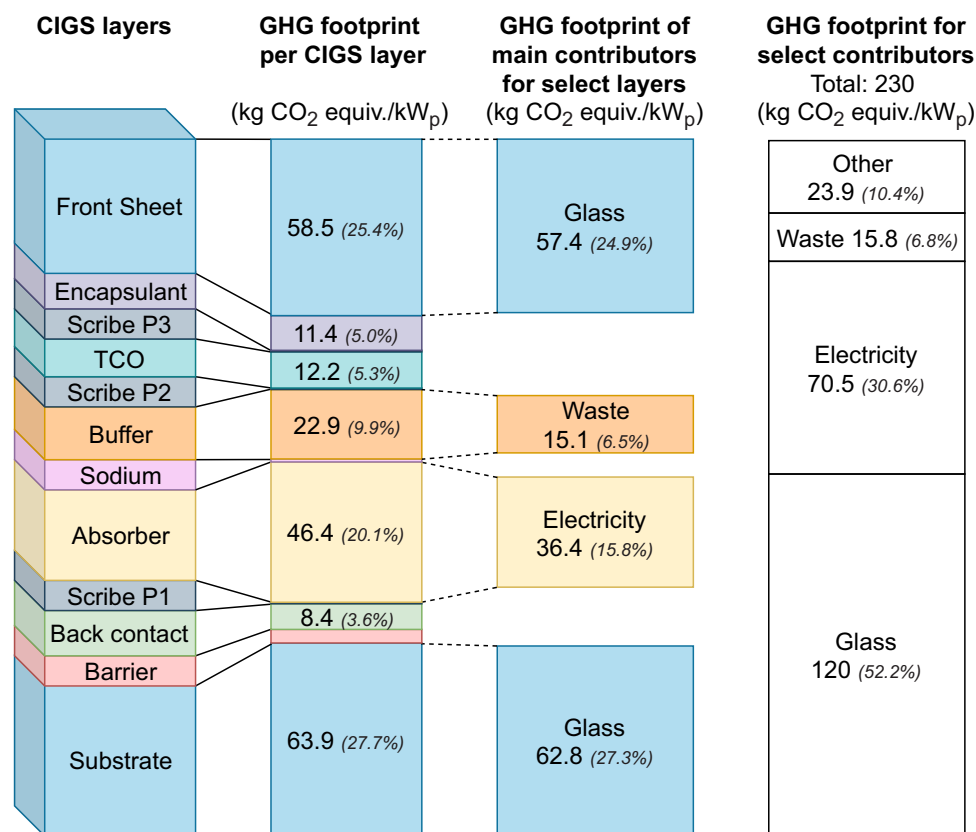


FIGURE 4 Results for the impact assessment of the pilot produced CIGS laminate. Percentages in parentheses represent the shares of each layer or material, relative to the total GHG footprint of 230 kg CO₂ equiv./kW_p of pilot produced CIGS laminate. CIGS, copper, indium, gallium, (di)selenide; TCO, transparent conductive oxide. Numerical data for these bar graphs are available in Table S2-1 of Supporting Information S2

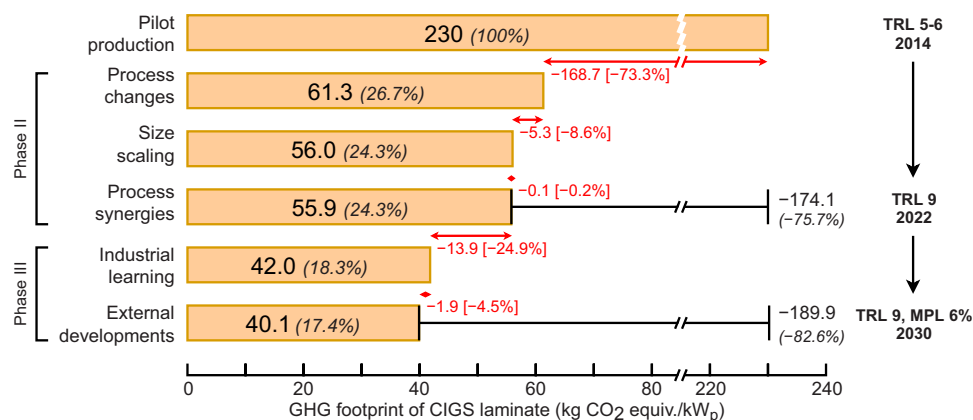


FIGURE 5 Results for the impact assessment of the CIGS laminate production process at different stages of development. Percentages in parentheses represent the shares of GHG footprint, relative to the total GHG footprint of 230 kg CO₂ equiv./kW_p of pilot produced CIGS laminate. The red values indicate absolute reductions in GHG footprint for each consecutive development step. Percentages in brackets specify the relative difference between two consecutive development steps. The crossbars indicate reductions in GHG footprint for the product at TRL 9 (end of phase II) and for the product in 2030 (end of phase III). CIGS, copper, indium, gallium, (di)selenide

4 | DISCUSSION

4.1 | Evaluation of the systematic approach

Phase I of our systematic approach to evaluate the future environmental impacts of emerging technologies can be seen as an extension of the goal and scope definition of a conventional LCA in which an analysis of TRL and MPL can support the choice of changes in the modeling of system and

impacts. Phases II and III are an extension of the inventory analysis of conventional LCA in which experience mechanism toward technology and manufacturing readiness (phase II) and at the industrial production level (phase III) are addressed. The development mechanisms of phases II and III will most likely not be equally important for every prospective LCA. Future studies are required to better understand whether certain development mechanisms are systematically more important than others.

Availability of in-house data enabled the case study of a pilot scale process, while available roadmaps enabled the modeling of estimated future technological developments. These types of data are typically scarce, especially for technologies at a lower TRL. Collaboration with technology experts, as recommended by Villares et al. (2017), was indeed found to be of great help for the formulation of a representative baseline case and development scenario for the case study. In our proposed approach, knowledge from experts is particularly invaluable when identifying or verifying likely process changes and process synergies. On the other hand, the inclusion of size scaling, industrial learning, and external developments should ideally be based on analytic quantitative models for reproducibility. Publicly available datasets with known size scaling and environmental experience factors could expedite their application in prospective LCAs and improve consistency between studies.

The application of environmental experience curves has been mentioned as an interesting research opportunity in several recent prospective LCA studies (Arvidsson et al., 2017; Buyle et al., 2019; van der Giesen et al., 2020). It has therefore been included in our proposed approach for conducting prospective LCA and a method of application has been successfully demonstrated. However, the reliability and representativeness of environmental experience curves has yet to be proven, since little research has been conducted on this specific topic. For instance, applications are typically restricted to cumulative energy demand (e.g., Görig & Breyer, 2016; Louwen, van Sark, Faaij, & Schropp, 2016; Ramírez & Worrell, 2006) and GHG emissions (e.g., Bergesen & Suh, 2016; Caduff et al., 2012; Kätelhön, von der Assen, Suh, Jung, & Bardow, 2015; Louwen et al., 2016) and it is unclear whether other impact categories show similar log-linear correlation with cumulative production. Furthermore, environmental experience curves are available for a limited set of products and materials. Further research into environmental experience curves is therefore required.

Granted that the concept of environmental experience curves can be applied to any impact category, our proposed approach could be applied in prospective LCA beyond establishing only the GHG footprint. However, one should note that emerging technologies can lead to novel environmental impacts that are currently not covered by any available LCIA method (Arvidsson et al., 2017; Cucurachi et al., 2018; Hetherington et al., 2014; Moni et al., 2020; Thonemann et al., 2020; van der Giesen et al., 2020). While the development of new LCIA methods can be essential to prospective LCA studies of certain emerging technologies, it is left outside the scope of our analysis for reasons of feasibility.

Next to analyzing development steps for the technology itself, a first effort was taken in this paper to include exogenous developments, that is, the change in GHG intensity of electricity generation. In this context, Cooper & Gutowski (2020) complemented prospective LCA by including the technology's current and future addressable market size as well as technology diffusion, technology displacement, and rebound effects. These type of additional aspects, such as the influence the emerging technology itself has on the impact of others (e.g., electricity generation by the produced CIGS panels), on the market (e.g., is consumption enhanced or are other technologies replaced), or on consumer behavior (e.g., whether it could trigger rebound effects), were not included at the current stage due to lack of data.

The application of our approach to project environmental impacts of emerging technologies requires assumptions which introduce uncertainties that influence the final results of the prospective LCA. Although we did not perform an uncertainty analysis ourselves, the quantification and reporting of uncertainty is clearly an important topic in LCA. Many different methods for uncertainty quantification have been developed which can also be considered for prospective LCA. Some examples from the literature include Likert's scale of (dis)similarities (Walczak, Hutchins, & Dornfeld, 2014), Monte Carlo simulations (Mann, de Wild-Scholten, Fthenakis, van Sark, & Sinke, 2013; Parisi, Maranghi, & Basosi, 2014; Ravikumar, Seager, Cucurachi, Prado, & Mutel, 2018), and sensitivity analysis (Mann et al., 2013; Raugei, Bargigli, & Ulgiati, 2007). Of these, Monte Carlo simulations could be particularly useful in uncertainty analyses of the applied size scaling factor and environmental experience rate in the size scaling and industrial learning steps of the proposed approach.

4.2 | Case study results

It is important to note that the scope and functional unit applied in our case study limit the comparison of our results with those reported in the literature. Our case study considers the production process for CIGS laminate and excludes the use and end-of-life phases of this product. Comparable studies in the literature did take into account the use phase, so for the comparison of results, functional units had to be converted from kWh to kW_p based on reported performance parameters. These parameters were annual electricity output per watt peak and lifetime (Stamford & Azapagic, 2019), photovoltaic efficiency and lifetime electricity output per area (Amarakoon et al., 2018), or annual solar irradiance, photovoltaic efficiency, lifetime, performance ratio, and degradation rate (Bergesen, Heath, Gibon, & Suh, 2014; Dominguez-Ramos, Held, Aldaco, Fischer, & Irabien, 2010). When modeling future developments for the CIGS production process, the scope of our case study makes it impossible to take into account changes in the lifetime of the CIGS laminate, which is a relevant indicator of progress in the PV industry. The estimated GHG footprints in 2030 from our case study should thus be considered indicative rather than an absolute outcome. In fact, Villares et al. (2017) argued that performing LCA in an ex ante context "does not permit reaching an environmental assessment which can be considered an accurate result." This is especially true for our case study, since the set of modeled developments was restricted, to allow for a clear and concise demonstration of the

proposed approach. While the narrow scope and selected functional unit enabled a simplified case study based on in-house available data, a more comprehensive cradle-to-grave assessment with a functional unit of kWh would promote a more direct comparison with available literature.

The GHG footprint of 230 kg CO₂ equiv./kW_p for the pilot CIGS production in our case study was compared to values reported in the literature for case studies using primary data. A recent study in Stamford and Azapagic (2019) used industry data from Solibro GmbH in Germany for the production of CIGS panels on rigid glass substrates, with production data covering a 2015–2018 period. Larger consumptions of electricity, glass, and CIGS absorber were reported in the LCI of this production process. Accounting for these differences, the GHG footprint of the Solibro production process was approximately 280 kg CO₂ equiv./kW_p, which is 22% higher than found in our case study. The contribution of balance of system (BoS) and framing were excluded, but contributions of additional differences, such as the inclusion of a junction box and the application of a different chemical bath deposition method, could not be inferred from the available data. Another recent study from Amarakoon et al. (2018) assessed prototype/pilot production of flexible CIGS panels by the PVMC R&D facility in New York State for 2014. The GHG footprint for a CIGS laminate with integrated cell interconnection was approximately 227 kg CO₂ equiv./kW_p. No comprehensive LCI was reported, which complicated comparison of the modeling approaches and resulting study outcomes. A more extensive description of the comparison between our case study and these two case studies in the literature is provided in Section 5 of Supporting Information S1.

The estimated 83% reduction in GHG footprint for the CIGS laminate production to 40.1 kg CO₂ equiv./kW_p in 2030 was compared to predictions for 2030 reported in two other prospective LCA studies for CIGS. Dominguez-Ramos et al. (2010) used production data included inecoinvent 2.0 and considered a general 20% reduction in material and energy requirements per produced unit over the period from 2007 to 2030, which was attributed to unspecified improvements in manufacturing processes. An increase in photovoltaic efficiency and performance ratio was also included over this period. The GHG footprint was estimated to drop by 45% from 1,312 to 719 kg CO₂ equiv./kW_p as a result of these modeled changes. The reported modeling methods do not include the full scope of technological developments encompassed in our proposed systematic approach, thereby likely underestimating the future reduction options in GHG footprint. Bergesen et al. (2014) used data from the NREL manufacturing cost model, which was compiled through collaboration with industry partners. For the period from 2010 to 2030, the GHG footprint was projected to drop by 68% from 941 to 302 kg CO₂ equiv./kW_p for roof mounted systems and by 69% from 806 to 254 kg CO₂ equiv./kW_p for ground mounted systems. For the latter, these reductions are attributed to BoS recycling (8%), module photovoltaic efficiency increases (29%), dematerialization (10%), and changes in the background economy (22%) assuming the IEA's BLUE Map development scenario. This case study included process changes and external developments as defined in our proposed approach, but did not account for size scaling, process synergies, or industrial learning for the production process. For both case studies, the contribution of the production process to the estimated lifetime GHG footprint could not be inferred from reported data. A more extensive description of the comparison between our case study and these two prospective case studies in the literature is provided in Section 5 of Supporting Information S1.

5 | CONCLUSIONS AND OUTLOOK

In this paper we presented a novel approach to perform prospective LCAs, which can be used to extend existing guidelines for conducting LCA, and we successfully demonstrated the application of this approach on a CIGS case study. Via direct collaboration with PV engineering experts, we were able to analyze each step of technological development and could quantify the importance of these steps with respect to the overall decrease in GHG footprint.

To further enhance the feasibility of applying the proposed systematic approach, we highly recommend the development of open source databases, containing process-specific information on process alternatives, size scaling, common production line synergies, and industrial learning. Examples of this type of information can be readily found in the literature for size scaling (Caduff et al., 2011; Caduff et al., 2012; Caduff et al., 2014) and experience rates (Bergesen & Suh, 2016; Caduff et al., 2012). These databases should preferably include the TRLs, MRLs, MPLs, market sizes, and cumulative production of emerging and incumbent technologies and their respective components. As discussed by Pauliuk, Majeau-Bettez, Mutel, Steubing, and Stadler (2015), the subsequent collection, storage, and sharing of information could be facilitated by existing platforms, such as the UNEP/SETAC Life Cycle Initiative.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

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