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Practical solutions for *ex-ante* LCA illustrated by emerging PV technologies

Stefano Cucurachi[1]
Carlos Felipe Blanco[1]

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[1] Institute of Environmental Sciences (CML), Leiden University, The Netherlands, s.cucurachi@cml.leidenuniv.nl, c.f.blanco@cml.leidenuniv.nl

Introduction

In this paper, we discuss practical challenges in *ex-ante* life cycle assessment (LCA) of emerging technologies, i.e., barriers to hands-on implementation, as opposed to the conceptual challenges that recent contributions to the literature have been focusing on (see Giesen et al., 2020; Thonemann et al., 2020; Villares et al., 2017). We will illustrate the discussion with the case of emerging photovoltaics (PV), namely multijunction III-V/silicon tandem cell (III-V/Si). This case application helps structure the *ex-ante* LCA exercise and highlights the challenges of applying LCA early on in technology development, while providing sufficient general elements that apply to other emerging technologies.[2]

Written from the perspective of LCA analysts, the paper is organized around the LCA method. LCAs can be conducted at various stages of a technology development process, requiring different types of information at the various stages. By illustrating with the case study of emerging photovoltaics, the paper explores the importance of product performance optimization during technological development, and how it is directly linked to environmental performance during the use phase. It also demonstrates how the design and manufacturing choices that technology developers are confronted with can greatly influence environmental performance over the future product's life cycle. The approach that emerges is one in which the LCA method remains flexible throughout the technology development process to accommodate its dynamic nature and the numerous uncertainties inherent in it.

1.

Why we need *ex-ante* LCA

LCA is the method of choice to assess product and service systems that span the global economy and trigger environmental trade-offs across multiple impact pathways. For several decades now, LCA has been used to quantify the environmental impacts of products or services across their full life cycle, from the extraction of raw materials up to the end-of-life (EOL), and across a wide range of impact categories, from climate change to toxicity and acidification (Hellweg & Canals, 2014). A series of ISO standards (ISO, 2006b, 2006a) formalised the use and application of LCA. These LCA studies have mostly been *ex-post* assessments of well-defined systems, namely systems for which sufficient data and knowledge were available, given that the systems have already been operating at an industrial scale. *Ex-post* LCA studies can guide decision-makers and consumers on the environmental hotspots in the life cycle of a product system and can be used to compare environmental benefits and trade-offs vis-à-vis an incumbent product system performing a similar function. While useful for decision-makers, *ex-post* LCA studies can have limited use when they call for changes that are likely to be costly or unfeasible (Cucurachi et al., 2018).

Assessing a system that is still being designed or that is still in development has the advantage that changes are still possible. A designer of a novel or emerging technology, for instance, would have the choice to use the results of an LCA study to avoid designs that require manufacturing processes or features that lead to an increase in environmental sustainability impacts from a sustainability perspective. Furthermore, *ex-ante* LCA accounts for the process optimizations required to mass-produce and deploy an emerging technology at an industrial scale (Bergerson et al., 2020; Giesen et al., 2020). Additional advantages of performing an *ex-ante* LCA are the close collaboration with technology developers and other stakeholders, the ability to put claims of environmental sustainability to early scrutiny, to support early design improvements and sound investments with information about potential large-scale environmental impacts at hand, to avoid technological lock-ins, to identify early hotspots or comparative advantages/disadvantages, and to warn decision-makers about critical material and process choices. *Ex-ante* LCA has been gaining traction, and scholars and practitioners have been working in the past few years to develop new methods that are suited to assess emerging systems and technologies (we refer the reader to Bergerson et al. (2020) and Giesen et al. (2020) for the classification of alternative modes of LCA to assess systems prospectively).

[2] See the paper written for the ESET project by Christian Moretti, "Ensuring the environmental sustainability of emerging technologies applications using bio-based residues" (2022).

2.

Background: *Ex-ante* challenges

Ex-ante LCA studies fall into the methodological quandary known as the Collingridge dilemma (Buckley et al., 2017), which postulates that impacts cannot be easily predicted until the technology is extensively developed and widely used, while control or change is difficult when the technology has become entrenched.

Several scholars have highlighted the different nature and challenges of conducting an *ex-ante* LCA compared to the standard practice of LCA, as defined by the ISO 14040 standards (see Guinée, 2001 for an operational guide to the ISO standards). Technology-specific guidelines are also available. For example, readers can consult Langhorst et al. (2022) for guidelines on the LCA of CO_2 utilization technologies and the report published by the European Commission's Knowledge Centre for Bioeconomy (2022) for the application of *ex-ante* LCA to bio-based systems. In the next sections, we will assess some of the challenges in turn. Here, we provide a short review of the challenges and the phases of LCA in the order of which they need to be tackled.

Several aspects of the goal and scope phase, the initial phase of any LCA study, become critically important to define for emerging technologies due to the need to understand the product's ultimate *functional performance*, i.e., how much service it can deliver or needs it can satisfy per unit of product and under what conditions. By calculating impacts on the basis of a specific *functional unit*, the analyst is able to capture trade-offs between the *functional performance* of the system and the related environmental impacts. Giesen and co-authors (2020) stress the difficulties in defining a functional unit for technologies that are yet to be implemented on the market, as well as in finding a relevant incumbent technology performing a similar function for benchmarking (see also Arvidsson et al., 2017; Hetherington et al., 2014; Wender & Seager, 2011). This challenge of comparing an emerging vs. an incumbent technology is highlighted by several review studies (Arvidsson et al., 2017; Hetherington et al., 2014; Moni et al., 2020; Thonemann et al., 2020). A screening of alternatives should be conducted (Langhorst et al., 2022), and Moni and co-authors (2020) suggest defining and assessing multiple functional units and their alternatives, if needed, so that the full spectrum of potential alternatives can be covered. The identification of the functional unit(s) for the system under assessment is also strictly connected to the expectation of the developer of an emerging technology regarding the functional performance of the system both in the lab and at an industrial scale. An important decision that the analyst needs to make during the goal and scope phase of LCA relates to the identification of the system boundaries of the *ex-ante* study. System boundaries set the criteria and specify which unit processes are part of the product system (Thonemann et al., 2020). When assessing alternative systems performing a similar function, but which are at different technology readiness levels (TRLs), the system boundaries should be as broad as possible and must be harmonized between alternatives. A clear point of attention regards the EOL of emerging technologies, and whether the EOL should be included in the assessment given the uncertainty of which EOL will become available in the future.

During the life cycle inventory (LCI) phase, the analyst faces challenges related to data availability and coverage (Giesen et al., 2020; Moni et al., 2020; Thonemann et al., 2020). This mainly concerns data on material and energy inputs and outputs (flows) in all processes that will be part of the product/service's life cycle, and which ultimately trigger the environmental impacts. Data available in standard LCA databases might be obsolete, unavailable, or not representative, thus requiring the analyst to rely on scenarios, proxies, or gap-filling strategies. As for the specific technology under assessment, the analyst may face the challenge of modelling processes that are still at the lab scale, and that are bound to change should the technology penetrate the market and become industrially available. A parametrized system, where inputs/outputs are expressed as a function of variable parameters, may be better suited in conducting an *ex-ante* assessment (Blanco, Cucurachi, Guinée, et al., 2020). Additionally, upscaling techniques may be used to upscale processes from lab to industrial scale (Piccinno et al., 2016).

The life cycle impact assessment (LCIA) is dedicated to the characterization of potential impacts from the system of interconnected processes inventoried at the LCI stage. This is generally done by multiplying the aggregated input/output exchanges of materials and energy with the environment by characterization factors that quantify the impact resulting from each exchange. Standard characterization models used at the LCIA phase may not be fully suited to assess novel materials in emerging technologies, thus leaving unclassified flows and impacts as a result (Giesen et al., 2020). Due to a lack of data, such unclassified flows and results leave the decision-maker with a false sense of confidence about the realistic performance of the emerging technology under assessment (we further refer the reader to Moni et al., 2020).

In the final interpretation phase, the analyst evaluates the results of the study and assesses the implications of modelling choices on the results and the potential impacts of uncertainty and assumptions on the results of the study. In an *ex-ante* LCA study, scenario techniques (Bisinella et al., 2021) and advanced techniques of uncertainty and global sensitivity analysis aid the analyst in stress-testing the assumptions in the system and identifying the relevant inputs in the model that are potential drivers of uncertainty and key to make an informed decision on the system under assessment.

In the remainder of this paper, we discuss the above challenges in more detail and use the case of an emerging solar PV technology, the multijunction III-V/silicon tandem solar cell, to illustrate the following practical strategies to overcome the challenges:

1. Parametrized use-phase modelling (goal and scope phase)
2. Upscaling based on process engineering principles (LCI phase)
3. Expert elicitation (LCI phase)
4. Modelling technological pathways (LCI phase)
5. Using future background scenario LCI databases (LCI phase)
6. Assessing future impacts (LCIA phase)
7. Modelling EOL scenarios (goal and scope, and LCI phases)
8. Recognizing what matters in the LCA model (interpretation phase)

2.1 Case study of emerging photovoltaics

Crystalline silicon cells (c-Si) have been dominating the photovoltaic electricity (PV) market for over two decades, largely due to the availability and low cost of silicon and their relatively good performance in converting energy from sunlight. Industrially available c-Si cells today have conversion efficiencies of ca. 22%, while the record-holding lab prototypes are pushing towards the thermodynamic limit of 29.4% (Ehrler et al., 2020). Cost reduction has been exponential, reaching $0.20/Wp in 2020 (Benda & Černá, 2020). But after decades of research and development (R&D), marginal increases in c-Si efficiency and decreases in cost are more difficult to attain. Still, solar PV is expected to be a key player in the energy transition, and the most optimistic scenarios see installed capacity reaching 70 TW in 2050, up from 760 GW in 2020 (Jaxa-Rozen & Trutnevyte, 2021). In such a future, the market dominance of c-Si may be challenged by higher-efficiency cells if they can achieve a lower cost per watt. The emerging PV landscape is dynamic and diverse, with many novel combinations of materials and processing methods being proposed to achieve the lowest cost-per-watt ratios. At the same time, the focus on the cost per kW ratio could distract from the original goal of reducing the environmental burdens of energy systems. Emerging PV is, therefore, a very well-suited and justified domain for the application of *ex-ante* LCA.

The multijunction III-V/silicon tandem cell (III-V/Si) concept is an emerging PV technology that combines c-Si bottom cells with top absorber layers made from group III-V materials (gallium, indium, arsenide and phosphide) (Cariou et al., 2018). This combination allows such cells to reach conversion efficiencies well beyond c-Si's theoretical limit. With significantly less time and resources invested in R&D, III-V/Si cell efficiencies close to 36% have already been demonstrated at the lab scale (Essig et al., 2017). Recent R&D efforts have targeted potential pathways to improve cost and environmental competitiveness via more efficient III-V layer deposition, enhanced waste treatment, recycling of metals, and low-cost preparation of the c-Si growth substrate (Blanco, Cucurachi, Dimroth, et al., 2020; Fraunhofer ISE, n.d.). In this paper, we use such advancements to illustrate the challenges of applying LCA to an evolving system at a low TRL.

3. Goal and scope

During the goal and scope definition phase, important choices are made, and boundary conditions are defined for conducting an LCA study. The objective of an *ex-ante* LCA is to quantify the future environmental impacts of an emerging technology (Moni et al., 2020), e.g., to require funding or benchmark a system in comparison to an alternative. In comparative studies, the emerging technology is frequently compared to an incumbent technology, defined as the system in the technology landscape that performs a similar function as that of the emerging technology (Giesen et al., 2020). While in conventional LCA the incumbent systems are typically well-defined (European Commission's Knowledge Centre, 2022), in an *ex-ante* LCA study the incumbent systems may become clearer to the analyst only as the technology evolves, thus after iterations of the assessment are carried out in close coordination with technology developers. This process could take years, making finding a balance between timeliness and accuracy challenging but necessary.

The transparent definition of a reference year for the analysis, geographical context and technological landscape allows for modelling scenarios that consider all the relevant operating conditions (see also Bisinella et al., 2021; European Commission's Knowledge Centre, 2022). It is recommended at this stage that the analyst formulates the expected delay until there is industrial production, together with the specific TRL of the system under assessment (Moni et al., 2020). In the case of low TRL levels, the system is considered to be in the conceptual development phase and, thus, extensive process changes are expected due to further research developments (Gavankar et al., 2012). In comparative assessment, it is important to account for the TRL of the emerging technology and the related incumbent technology and to discuss the implications of TRL on the potential performance of the systems.

3.1 Functional performance

Once the objective of the study is clearly defined, a functional unit (FU) can be defined, i.e., a "quantitative description of the service performance (the needs fulfilled) of the investigated product system(s)" (Rebitzer et al., 2004). Challenges in *ex-ante* LCA may arise regarding the precise identification of the function of the technology under assessment. At the earliest stages of innovation, it might be challenging for the analyst and technology developer to fully define the ultimate function of emerging technology, and this may be influenced by future consumer behaviour, i.e., how they use the technology. It is also possible that multiple functions may be identified and studied, and they may require comparison with multiple incumbent technologies, e.g., batteries may be used for frequency/voltage regulation of the energy grid or for energy storage in residential units.

Another key challenge is that the functional performance (i.e., the efficiency in delivering the required function) of the technology, once it is market-ready, is often uncertain. Performance improvement is often the main target of R&D, and performance gradually (sometimes significantly) improves as the technology progresses from one TRL to the next (see Table 1).

Table 1 | Examples of emerging technologies typically evaluated in *ex-ante* LCA and how their expected functional performance can evolve throughout R&D

Technology	Functional unit example	Example performance improvements targeted in R&D
PV panels	1 kWh generated electricity	Increase panel conversion efficiency, reduce degradation
Batteries	1 kWh delivered electricity	Increase roundtrip efficiency, increase cycle life
Electric vehicles	1 km transport	Increase engine efficiency, increase components' lifetime
Carbon capture and storage	1 kg captured carbon	Increase adsorber efficiency and lifetime
Bioproducts	1 kg biomass	Increase bioreactor yield

Functional performance — and its determining factors — are often the most influential unresolved aspects for LCAs of emerging technologies. In an LCA model, the performance of a service (such as generating electricity, transporting passengers, or providing novel nutrition sources) is a use-phase activity that is downstream of most other activities in the value chain. Better performance will demand less from the upstream supply chain to deliver the same amount of service. Therefore, it is of the utmost importance that this aspect is carefully modelled and analysed via uncertainty and sensitivity analysis (see section 6).

As can be gathered from above, we recommend detailed modelling of functional performance aspects, which can then be subject to comprehensive uncertainty and sensitivity analyses (section 6). We also recommend erring on the side of over-parametrization rather than under-parametrization in this part of the model, as important opportunities for optimising designs for increased sustainability may be revealed.

Ex-ante practical strategy 1: Parametrized use-phase modelling

The relevance of functional performance is well illustrated by the case of emerging PV. For PV, the functional unit is often defined as "1 kWh (kilowatt-hour) of DC electricity generated by a photovoltaic module" (Directorate-General for the Environment of the European Commission, 2020). The key quantity of interest for calculating life cycle impacts is the size of the PV installation required to generate this amount of electricity. This size will depend on several performance-related factors, according to the formula:

$$A = E/(I \cdot \eta \cdot PR \cdot LT)$$

Where A is the size of the PV installation (in m²), E is the required electricity given by the FU (i.e., 1 kWh), I is the incoming solar irradiation ($kWh/m^2 \cdot a$), η is the panel's conversion efficiency, PR is a performance ratio expressed as a percentage, and LT is the expected useful lifetime of the panels, in years. Any performance improvement in conversion efficiency, performance ratio, or panel lifetime will proportionally reduce the installation size A required to generate 1 kWh of electricity, therefore reducing the consumption of materials and reducing the impacts of these materials per kWh of electricity generated.

Furthermore, solar cells can be expected to degrade over time, lowering their efficiency (η). Degradation is thus an additional key performance factor. The Product Environmental Footprint Category Rules (PEFCR) put forth by the European Union prescribe a degradation rate of 0.7% each year for all PV technologies, only to be revised if a different value can be substantiated by long-term testing (> 10 years). In the context of emerging PV technologies, this is naturally not feasible. Yet our goal of understanding *potential* impacts and improvement pathways requires an analysis of *potential* performance, especially if improved solar cell efficiency and stability (and/or panel lifetime) are key features of the PV technology being evaluated.

The III-V/Si technology can offer important improvements in several of the factors which should be captured by an *ex-ante* LCA. Figure 1 shows the comparative LCA impacts for III-V/Si PV vs c-Si, taking the PEFCR recommended baseline values: annual irradiance (1700 kWh/m²), PV system lifetime (30 years), performance ratio for roof-mounted systems (75%) and a degradation rate of 0.7% per year. The initial conversion efficiency of 27% is taken based on what has been achieved to date for III-V/Si. Technically feasible and foreseeable performance optimizations are assessed by extending lifetime to 35 years, increasing efficiency to 30%, reducing degradation to 0.5%/year and increasing the performance ratio to 80% (see Figure 1: LT_opt, Eff_opt, Deg_opt, PR_opt, respectively).

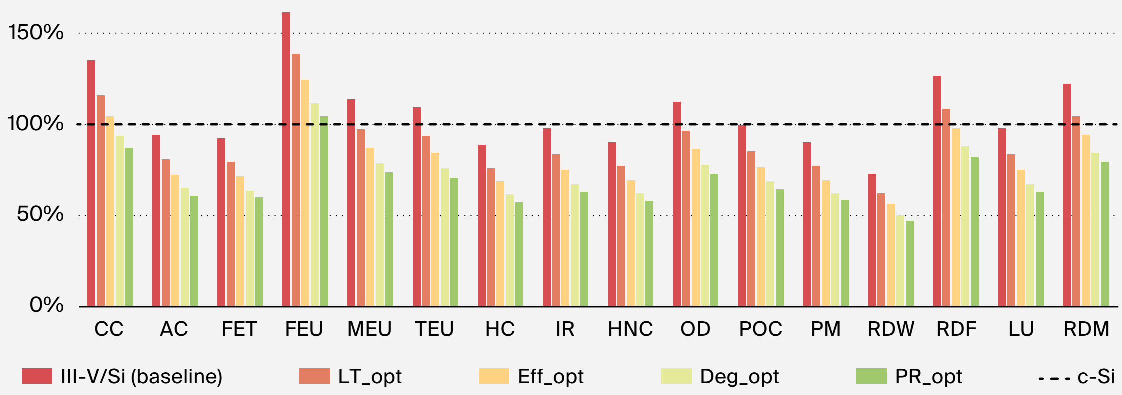

Figure 1 | Comparative impact results of III-V/Si future scenarios compared to the reference c-Si system with an improved panel conversion efficiency of 30%, degradation rate of 0.5% per year, extended lifetime of 35 years and performance ratio of 80%. CC: climate change; AC: acidification; FET: freshwater ecotoxicity; FEU: freshwater eutrophication; MEU: marine eutrophication; TEU: terrestrial eutrophication; HC: human toxicity, cancer effects; IRH: ionising radiation; HNC: human toxicity, non-cancer effects; OD: stratospheric ozone depletion; POC: photochemical ozone formation; PM: particulate matter; WRD: water resource depletion; RDF: fossil resource depletion; LU: land use; RDM: mineral resource depletion.

4.

Future LCI: Foregrounds and backgrounds

The emerging technology system and incumbent system/systems under assessment can be defined as the foreground system, i.e., the part of the system that the analysts model themselves. For the case of emerging technologies, the foreground system is also typically under the direct control of the technology developer with whom the LCA analyst collaborates, meaning that specific processes in the emerging technology product system could be influenced and changed given adequate resources and guarantees of acceptable trade-offs on the functional performance. For example, nitrogen could be used instead of hydrogen when non-reactive gas streams are required in a chemical processing step, should the LCA analyst signal an environmental preference for the first option as compared to the latter.

The technological context in which the emerging technology and incumbent technology (or technologies) are embedded can be defined as the background system, i.e., the part of the system for which LCA analysts typically use LCI databases (e.g., ecoinvent Wernet et al., 2016). An example of unit processes in the background is the service of electricity provision from the grid, which does influence the performance of the emerging technology, but depends on policy decisions and a country's macro-economic context.

While modelling choices related to the foreground and background systems are decided upon during the goal and scope phase, they do have an impact on the inventory data used at the LCI phase. The literature suggests avoiding temporal mismatches between foreground systems and background systems (Arvidsson et al., 2017; Giesen et al., 2020; Mendoza Beltran et al., 2020; Thonemann et al., 2020), although this is often not possible.

4.1 Upscaling the foreground

Lab- and pilot-scale processes are often how technologies are built up and transformed during R&D. However, these processes are highly inefficient in their use of energy and materials, and as a result, would likely have disproportionate environmental impacts if introduced in an LCA model. Given that such processes will not be used to manufacture the technology at an industrial scale, the results of a lab/pilot-scale LCA model could provide, at best, limited insight and, at worst, distorted conclusions as to the future environmental performance of the technology. One of the foremost challenges encountered by *ex-ante* LCA practitioners is, thus, the lack of knowledge of how each lab/pilot-scale process being tested by technology developers will be optimized for industrial mass production.

Ex-ante practical strategy 2: Upscaling based on process engineering principles

Piccinno et al. (2016) offer excellent guidance for upscaling chemical processes in LCA models, based on process engineering principles and well-known practices in the chemical industries. The approach can be illustrated with the front metal contacts (fingers and busbars) of the III-V/Si cells case study. Current industry practice is to screen-print the metal contacts using silver paste. However, silver is expensive and is ranked high vs. other metals in terms of potential ecotoxicity impacts in LCA impact assessment models. A proposed innovation is to replace it with copper nano ink, with the caveat that copper ink must be sintered (dried and consolidated) in an oxygen-free environment to avoid damage. This environment is provided by a constant flow of nitrogen gas with formic acid (Hermerschmidt et al., 2018). A laboratory setup for this sintering step is depicted in Figure 2.

An LCA of III-V/Si including this lab-scale process would quickly raise a flag since sintering would introduce climate change impacts orders of magnitude larger than all other processes and components of the PV installation. Most of the burden would be traced to the large consumption of formic acid per solar cell processed (Figure 3, top). But this is an unrealistic representation, as such a process is by no means scalable. Following the guidance of Piccinno et al. (2016), we establish that the formic acid is mostly non-reacting and therefore would likely be recirculated in an industrial setting, greatly reducing the environmental burden of this step (Figure 3, bottom). The reader is referred to Piccinno et al. (2016) for additional strategies regarding the consumption of energy and reactants, as well as reactor geometry and waste handling.

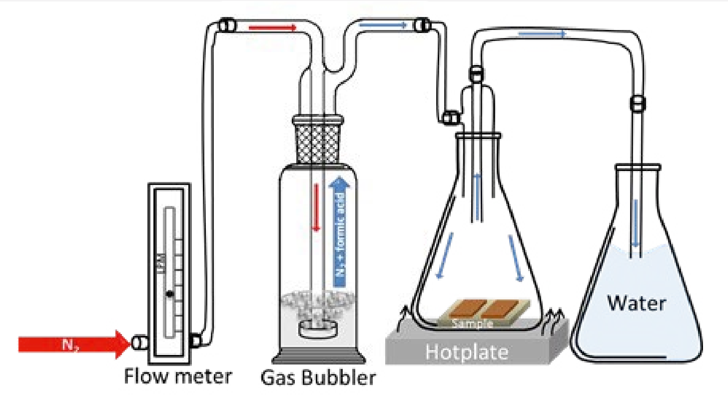

Figure 2 | Lab-scale demonstration of copper ink sintering of front contacts in sample 1 cm² sized solar cells (credits: Mirella El Gemayel).

Figure 3 | Process contributions to climate change impacts of III-V/Si panels with lab-scale (top) and industrial-scale (bottom) sintering of front contacts (left) and upscaled sintering (right) (credits: Mirella El Gemayel).

Ex-ante practical strategy 3: Expert elicitation for hotspots

A similar situation is encountered in the deposition step of PV cell fabrication, where the top III-V layers are placed on top of the silicon wafer (Blanco, Cucurachi, Dimroth, et al., 2020). With current technology, this deposition is done in metalorganic vapour phase epitaxy (MOVPE) reactors operating at high temperatures (> 900°C) with low throughputs (e.g., 31 round 4-inch wafers per 2.5-hour run). The combination of low-throughput and high-energy demand in a manufacturing step is likely to make it an LCA hotspot and is something for *ex-ante* practitioners to be on the watch for. This is confirmed for the III-V/Si case, as seen in Figure 3. Thousands of MOVPE reactors would be required to reach the targeted industrial-scale production capacity of billions of cells per year. The capital expenditure and operational costs of such a reactor fleet would render the III-V/Si technology technically and economically inviable. The MOVPE reaction will necessarily have to be optimized, and the question then is how to do so and to what extent.

In a European project in which the authors were involved (Fraunhofer ISE, n.d.), a focus group involving engineering experts was created to discuss what improvements are necessary and also feasible and foreseeable in the MOVPE process. The output of this expert elicitation was a roadmap with eight milestones, each representing an optimization of the MOVPE process needed to approach industrial-scale production and cost targets.

Table 2 | Description of future foreground scenarios for MOVPE optimization

Milestone	Description
III-V/Si P	Present MOVPE reactor configuration with a throughput of 31 small 4-inch round wafers per run and runtime of 2.5 h
M1	Change shape and size of wafer handled by the reactor to larger 156.75 x 156.75 mm square wafers
M2	Increase throughput to 50 wafers per run
M3	Reduce runtime to 1 h by minimizing intermediate steps and increasing some deposition rates
M4	Reduce runtime to 0.5 h by minimizing intermediate steps and increasing some deposition rates
M5	Increase reactor deposition efficiency from 50% to 60% (reduce III-V material consumption)
M6	Reduce equipment power load of MOVPE reactor from 15 kW to 5 kW
M7	Reduce cooling power load from 16 kW to 5 kW
M8	Reduce facilities ventilation power load from 39 kW to 20 kW

Recalculation of the LCA for each milestone showed that a combination of steps would suffice to achieve a comparative environmental advantage for the III-V/Si tandem cells (see Figure 4). This result is remarkable, considering that the incumbent c-Si cells are already mass-produced in assembly lines that handle > 5000 square wafers per hour. Such an approach can be replicated in additional contexts in which an LCA analyst is collaborating with technology developers early in R&D to elicit feasible technological roadmaps to assess via LCA. The reader is referred to (Morgan, 2014; O'Hagan, 2019; Wang et al., 2012) for in-depth descriptions of structured elicitation protocols.

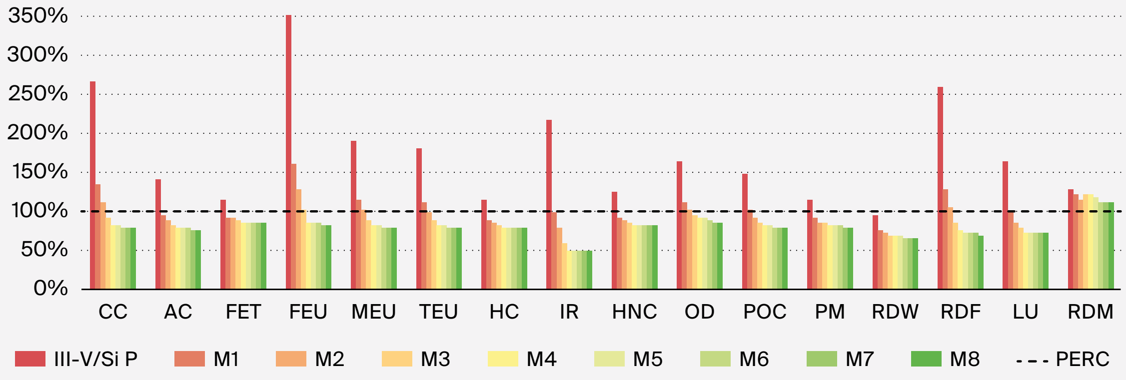

Figure 4 | Life cycle environmental impacts of generating 1 kWh with a III-V/Si tandem module on a slanted-roof installation, following MOVPE process optimizations M1–M8 (Table 2). Impacts are shown relative to incumbent c-Si modules (red dashed line = 100%). CC: climate change; AC: acidification; FET: freshwater ecotoxicity; FEU: freshwater eutrophication; MEU: marine eutrophication; TEU: terrestrial eutrophication; HC: human toxicity, cancer effects; IRH: ionising radiation; HNC: human toxicity, non-cancer effects; OD: stratospheric ozone depletion; POC: photochemical ozone formation; PM: particulate matter; WRD: water resource depletion; RDF: fossil resource depletion; LU: land use; RDM: mineral resource depletion

4.2 Projecting changes in the background

As technologies progress from TRL1 to 9 (usually 10+ years), background supply chains can also be expected to evolve. For example, most global scenarios agree that energy grids around the world will likely turn towards less carbon-intensive sources, and economies will become more circular, reducing waste and consumption of raw materials. The number of interconnected processes in any product's background can easily exceed 10,000. Background LCA databases such as ecoinvent (Wernet et al., 2016) take a long time to compile and update, and even the most current databases often reflect technologies from 5–10 years ago. However, a technology may be better situated to take advantage of background trends than the incumbent technology. For example, this would be the case if it uses a material with a better outlook towards recyclability and reusability in the future. If future recycling trends are expected to better incorporate the materials in novel technology designs, this competitive advantage should be captured by an *ex-ante* LCA.

The matter of static or outdated background data has received considerable attention from LCA practitioners in recent years. One of the first practical solutions was proposed by Mendoza-Beltran et al. (2020), who translated future scenarios from the Integrated Model to Assess the Global Environment (IMAGE) models, developed and maintained by PBL Netherlands Environmental Assessment Agency (Stehfest et al., 2014), into future background LCA databases. The implementation of Mendoza-Beltrán et al. (2020) is based on the Shared Socioeconomic Pathways (SSPs) scenarios, which represent five storylines on possible human development trajectories and global environmental change in the twenty-first century. For example, the SSP2 scenario, "medium challenges to mitigation and adaptation" represents a balanced, leaning toward conservative, view of how energy markets may evolve over the next decades (O'Neill et al., 2014, 2017; Riahi et al., 2017; Stehfest et al., 2014).

Figure 5 illustrates how applying the SSP2 background scenario affects the climate change impact scores of III-V/Si panels over the next three decades. The improvements are gradual, suggesting that the SSP2 scenario is indeed conservative. We note that the incumbent technology (PERC c-Si) will also be subject to the same changes in the background energy supplies; therefore, it is of value to reveal whether and to what extent these changes are more beneficial to the emerging technology than to the incumbent one.

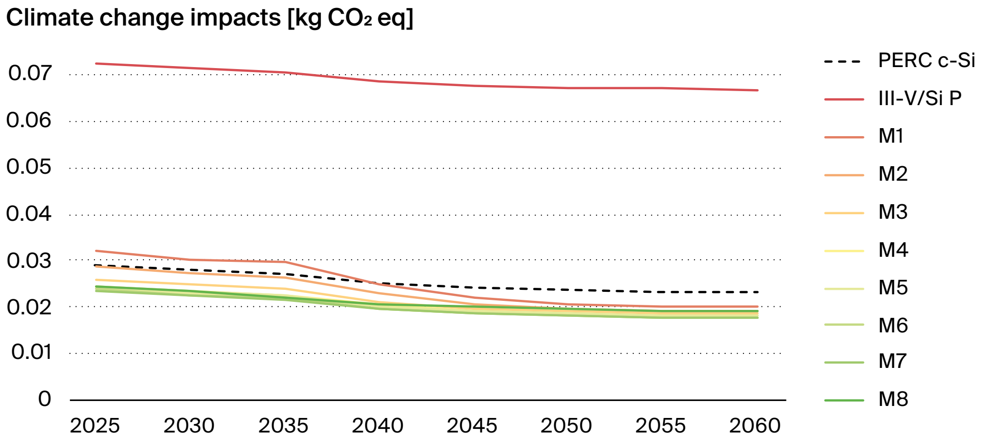

Figure 5 | Evolution of the climate change impact score of each future foreground scenario (milestones 1–8, see the previous section) modelled on future background SSP2-450 scenarios from IMAGE for the period 2020–2060

4.3 Competing processing and material alternatives

Another situation often encountered by *ex-ante* LCA analysts is that competing processing methods or materials will be tested by technology developers for different technology components. This will be evident in the foreground but may take place in background systems as well. The uncertainty, then, is not how much a given quantity such as energy consumption or processing runtime of a reactor will change, but whether an entirely different type of process, material, or equipment will be used to balance product performance with industrial scalability. Insofar as these decisions are not resolved (which may only happen at higher TRLs), the LCA analyst is challenged with assessing and communicating the impacts of numerous possible technological configurations, which can quickly become impracticable.

Ex-ante practical strategy 4: Defining and modelling technological pathways

Blanco et al. (2020) propose a probabilistic method for incorporating all possible combinations of process/materials choices (i.e., technological pathways) in a single LCA model, where the competing alternatives are selected stochastically in a Monte Carlo simulation according to their expected chances of success. The output of such a model (i.e., the impact score) is in the form of a probability distribution rather than a single-point value. The approach can be visualized in Figure 6. The challenging aspect of this approach is justifying the expected chance of success that is given to each alternative. Here, the analyst can resort to expert elicitation protocols such as those applied in strategy 3. (Morgan, 2014; O'Hagan, 2019; Wang et al., 2012).

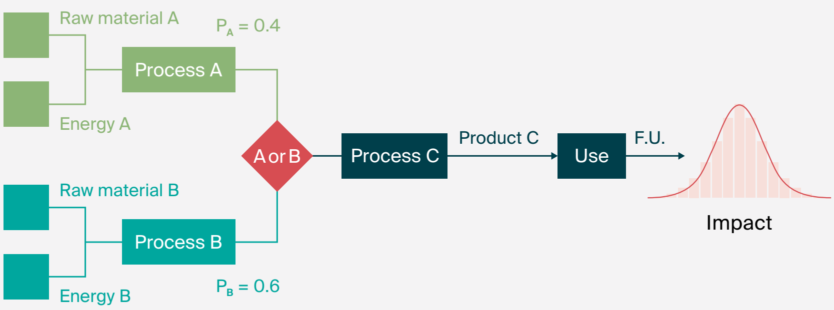

Figure 6 | Visualization of Monte Carlo propagation of competing for technological pathways.
P_A: expected chance of success of process A.
P_B: expected chance of success of process B

4.4 End-of-life treatment, emissions and impacts

Where the product or function of a technology (and its embedded system) serves a mature market, "cradle-to-gate" system boundaries may be appropriate for the goals of an LCA. However, emerging technologies may often provide a distinct product or service for which a market is not well established, which warrants careful consideration of market effects and the EOL phase (Bergerson et al., 2019). While a cradle-to-gate assessment of an emerging technology may require looking 10–15 years in the future, incorporating the EOL phase -which may take place 30 or more years later- really stretches the foresight capacity of the tools available to support LCA. Yet often the life cycle impacts of a technology are materialized in the EOL phase. This is especially the case for impacts such as ecotoxicity, acidification and eutrophication, which are triggered by chemical releases after incineration or landfilling of the technology's components. Other impacts, such as mineral resource depletion, will largely depend on the recyclability of such components, specifically if closed recycling loops are implemented. Emissions from waste streams in LCA are calculated from generic incineration/landfill models with a limited degree of product specificity (Wernet et al., 2016). Preserving a cause-effect link between the discarded product and its EOL emissions would require a specific emissions model to be developed, making this a very challenging aspect to model as no data can be collected for EOL situations, and recycling tests are seldom included in R&D programmes of novel technologies.

5. Future impacts: Novel materials and evolving landscapes

LCA allows for the characterization of impacts across a broad set of impact categories and regions of the globe, accounting for a broad range of emissions and their potential impacts. However, technology develops faster than LCIA models (Temizel-Sekeryan & Hicks, 2021). As highlighted by Giesen and co-authors (2020), it is important to realize that in *ex-ante* LCA studies, potential environmental impacts of new technologies are not automatically covered by the existing impact categories commonly used in *ex-post* LCA studies. As a result, applying the current set of impact categories and characterization models to a novel or emerging technology may result in

Ex-ante practical strategy 5: Modelling EOL scenarios

A simplified model can be developed for the EOL phase by considering the different components of the product in terms of their separability and expected economic value upon eventual recovery. Scenarios can then be developed for the recovery of economically attractive materials. The analyst is encouraged to report on the potential benefits (avoided impacts) from eventual product recovery separately, clearly stating all assumptions. Separation techniques applied to similar technologies may be reported in patents, giving clues as to the types of processing required, e.g., mechanical crushing, chemical, or thermal treatment. Here, it may be possible to highlight potential hotspots if high temperatures or hazardous chemicals are involved. As for recycling rejects or components that are not expected to become economically/technically recyclable, modelling specific emissions in a landfill or incineration facility will typically be beyond the scope of an LCA exercise. At the very least, it is useful to map out potential waste streams; if the waste is hazardous, it will likely be disposed of in an underground or security landfill, where foreseeable emissions are negligible. Incinerated wastes will produce solid waste, such as ash, which is sent to secure landfills or, in some cases, reintroduced in construction materials (Blasenbauer et al., 2020). Other types of waste may end up in less stringent landfills; for these cases, the analyst can assume a conservative scenario where an important fraction of the waste is eventually released to the surrounding soil environment.

unclassified and uncharacterized flows, due to a lack of models and data.

While unclassified and uncharacterized flows may be deemed negligible in a comparative context with shared background and foreground data, the lack of specific characterization models or characterization factors does have an impact on the possibility of intervening early in R&D to avoid environmental burdens (Giesen et al., 2020). An LCA analyst, for instance, would not be able to calculate the potential toxicity impacts of an emerging technology that would make use of a newly synthesized chemistry. This is due to the lack of an adequate characterization model able to characterize the cause-effect impact pathway of the said chemistry. The exclusion of these impacts, in such a case, could communicate to the decision-maker an artificial sense of safety[3], which would only be due to an imperfect assessment. In a comparative assessment, such a sense of safety may also shift the preference from the incumbent technology to the emerging one.

Ex-ante practical strategy 6: Updating characterization factors

The case of front metal innovation discussed in strategy 2 also provides a good illustration of the uncertain impacts of novel chemistries. While metallization inks for commercial c-Si PV cells are made of bulk silver paste, R&D is pushing towards the use of copper, as well as smaller particle sizes in the ink formulation, i.e., nano inks. Smaller particle sizes mean increased surface area, which has been linked to different intrinsic toxicity potentials than the bulk version of the same metal. Furthermore, nano-sized particles are subject to different transport mechanisms once released (e.g., particle aggregation), resulting in different fate and exposure factors. Thus, the databases with toxicity characterization factors, which were developed over several decades, may significantly under/overestimate the toxicity potential of novel material structures.

Updating toxicity characterization factors involves extensive lab testing and knowledge of a complex domain that is often beyond the reach of LCA practitioners. Fortunately, there is a growing body of literature aiming to fill this gap for nanomaterials, see e.g., Temizel-Sekeryan & Hicks (2021) (silver), Salieri et al. (2015) (TiO2), Miseljic & Olsen (2014) (silver and carbon nanotubes), Pini et al. (2016) (TiO2), Pu et al. (2016) (copper). The characterization factor for bulk copper releases in freshwater, according to the commonly used USEtox database is 194,000 CTU (comparative toxicity units) per kg of copper (2017). In contrast, Temizel-Sekeryan & Hicks propose a range between 2.19 × 103 and 2.34 × 105 CTU for silver nanoparticles. In both cases, the underlying uncertainties are very large and any treatment of these types of impacts must give uncertainty and variability due consideration. Alternatively, Song et al. (2017) propose assessing novel chemistries and materials by using artificial neural networks, thus using current knowledge of existing chemistries to assess in silico the impacts of novel chemistries and materials.

Another important consideration related to characterization factors in LCIA is that several impact categories calculate impacts relative to an evolving baseline. The most obvious examples are biotic and abiotic resource depletion, where the existing reserves are likely to change considerably in the time it takes for a technology to climb the technology development ladder from low TRL to TRL 9. A resource consumption now may be less “damaging” than the same consumption in 10 years. Baustert et al. (2022) have addressed this for the case of water scarcity in recent work, offering characterization factors projected to the year 2050. To our knowledge, no similar work has been conducted to date for minerals or other types of resources.

[3] See the paper written for the ESET project by Rainer Sachs, “Risk governance of emerging technologies: Learning from the past” (2022).

6.

Interpretation: Recent developments in uncertainty analysis and global sensitivity analysis

In recent years, the treatment of uncertainty in LCA has garnered increasing attention among LCA practitioners. While uncertainty analysis is mandated in the ISO 14040 standards for LCA (ISO, 2006b), it has been ignored in most studies or conducted only at a very superficial level. Current LCA databases have become much larger and more complex, and, as a result, the sources of uncertainty in the underlying data have increased significantly. Therefore, more comprehensive methods for analyzing and interpreting uncertainty in LCA models are needed, particularly when assessing emerging technologies.

7.

Outlook and generalization

Ex-ante LCA faces an overwhelming dearth of data, rapidly evolving technology designs, and limited time to adjust and reinterpret the models. In this paper, we used the case of emerging PV technologies to inventory, assess and provide practical guidance to tackle many challenges of conducting an LCA study at the earliest stages of technological innovation.

The traditional approach of only producing the assessments when a technology is fully developed, allowing for both models and data collection to be refined, has long been the standard of conventional *ex-post* assessments. Such an approach guarantees more accurate results at the expense of the risk of inaction because a technology is already

Ex-ante practical strategy 7: Recognizing what matters in the LCA model

Given the many different futures that can unfold, one of the key aspects of understanding and interpreting large uncertainties in an *ex-ante* LCA model is sensitivity analysis. Perhaps the most commonly applied method for sensitivity analysis in LCA is "one factor at a time" (OFAT) (Groen et al., 2017). OFAT analyses, which are a form of scenario analysis, consist of varying the values of selected input parameters and investigating how these variations are reflected in the model's output. OFAT analyses have several limitations, particularly their ad-hoc nature, given that the tested parameters are chosen subjectively by the practitioner.

A more thorough and systematic type of analysis is global sensitivity analysis (GSA) (Plischke et al., 2013), which systematically tests all of the model's uncertain input parameters and ranks them in terms of their contribution to the model output's uncertainty (e.g., contribution to variance). Several authors have argued strongly for the application of GSA in LCA, as it provides very valuable information on which input parameters should be investigated further to reduce the LCA model's output uncertainty (Cucurachi et al., 2016; Groen et al., 2017; Lacirignola et al., 2017; Ravikumar et al., 2018). Cucurachi and co-authors (2021) provide a protocol and software application to assess the importance of uncertain input parameters across all phases of an LCA model, including background and foreground contributions, and the use of the uncertain characterization model at the LCIA phase. The authors show, using a case study of III-V solar PV, that the proposed method and software application is suitable for the study of emerging technologies.

entrenched. We have shown that the *ex-ante* LCA alternative, combined with adequate screening tools and computational tools (e.g., for parametrization, uncertainty, GSA) can already guide decisions in the earlier phases of technology development. Such an approach requires close collaboration between LCA analysts and the relevant stakeholders, from the definition of the goal and scope of the analysis to all subsequent phases of LCA, including the interpretation of results. Similarly, substantial interdisciplinary work is required to build and extend the *ex-ante* LCA toolbox, calling for a necessary hybridization of LCA models with risk assessment models, technology and innovation theory, and data scientists, among other disciplinary experts.

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