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METHODS ARTICLE

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A framework for guiding safe and sustainable-by-design innovation

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Abstract

Assessing the safety and sustainability of novel technologies while they are still in the early research and development stages is the most effective way to avoid undesired outcomes. However, the journey from idea to market is highly uncertain and involves intensive trial and error as technology developers attempt to optimize material choices and product configurations. Designs evolve quickly, and assessing their risks and impacts while numerous factors remain undetermined is challenging. The standard practice is to evaluate a limited subset of scenarios that can guide design choices. However, selecting scenarios from hundreds of undetermined factors without a systematic sensitivity screening may leave out important improvement opportunities. To provide well-informed guidance, the evaluated scenarios should be selected based on factors that are most influential to the safety and sustainability impacts of the technology. We propose an approach that accomplishes this by incorporating a wide spectrum of undetermined factors, both intrinsic and extrinsic to the technology design. The assessment models are then screened for highly-sensitive factors using global sensitivity analysis. Strategies to reduce uncertainty on highly influential factors are proposed for subsequent iterations, and the residual factors for which uncertainty cannot be further reduced yet remain influential are selected as a basis for proposed "sensitive scenarios" and improvement roadmaps. We demonstrate the framework with an emerging photovoltaics case study. Over a hundred uncertain factors are reduced to less than five which, if optimized, would substantially improve the future safety and sustainability performance of the technology as well as reduce the uncertainty around it.

KEYWORDS
emerging technologies, innovation, prospective life cycle assessment, risk assessment, SSbD, uncertainty

1 INTRODUCTION

Safety and sustainability criteria are increasingly central in guiding policy decisions for supporting and regulating innovation (European Commission, 2022; OECD, 2022). To better support decision-making during early research and development (R&D) stages, safety and sustainability modelers have scrambled to propose diverse criteria and prospective approaches to life cycle assessment (LCA; Adrianto et al., 2021; Cucurachi et al., 2018) and human health and ecological risk assessment (Fernandez-Dacosta et al., 2019). The need for such prospective approaches has also been noted by the safe and sustainable-by-design (SSbD) framework for novel chemicals and materials being advanced by the Joint Research Centre of the European Commission (Caldeira et al., 2022) in response to a commission recommendation (European Commission, 2022). However, evaluating the safety and sustainability of novel materials and technologies poses a significant challenge. This challenge involves accounting for the uncertain evolution of technical, environmental, and socioeconomic factors—both intrinsic and extrinsic to the technologies—that will influence their future performance once deployed at a commercial scale (Fernandez-Dacosta et al., 2019; Frischknecht et al., 2009; Hetherington et al., 2014; van der Giesen et al., 2020; Villares et al., 2017).

Assessments of well-established mature technologies were already prone to inaccuracy and/or imprecision due to different forms of uncertainty and variability in the underlying models (Hertwich et al., 1999; Lloyd & Ries, 2008). A risk or impact estimate may deviate from its actual value due to spatial and temporal variability of the underlying processes, as well as imprecise or unavailable data regarding the technology's design and operational parameters (Huijbregts, 1998; Igos et al., 2019; Ramsey, 2009). Errors may also be introduced in environmental impact/risk assessment models, which are composed of mathematical relationships that can only offer limited approximations (Heijungs, 2020). At the very least, the impacts of existing technologies can—to some extent—be measured and validated empirically. Bereft of this possibility, even more uncertainty surrounds prospective assessments of novel technologies (Blanco et al., 2020).

To illustrate this challenge, we take the case of an emerging photovoltaic (PV) technology. At their end-of-life (EoL), the panels could be recycled, and the environmentally relevant or critical materials recovered, or they could be incinerated or disposed of in a landfill or underground waste deposit. The extent to which such materials are recovered will depend on economic factors along with regulatory concerns surrounding e-waste or supply risks. In this aspect, the ease and feasibility of future methods for physically separating the materials from the other panel constituents will also be determinant. The fate of these materials when released into the environment and the future exposures to humans and organisms may depend on evolving factors such as demographics and weather patterns. Recognizing the importance and heterogeneity of such uncertain factors in the LCA of emerging technologies, Miller and Keoleian (2015) proposed 10 factor types, grouped as *intrinsic* (e.g., changes in efficiency and functionality, infrastructure), *indirect* (e.g., supply chain effects, behavior change), and *external* (e.g., policy/regulatory effects).

The influence of such numerous and interrelated factors on the novel technologies' safety and sustainability performance once they reach the market will remain unknown until the assessments are conducted and complemented with sensitivity analysis (Hirt et al., 2020). A common strategy that has been widely applied to deal with uncertain factors of presupposed relevance is scenario analysis (Adrianto et al., 2021). This approach has been deemed to make the assessments more robust, especially in the presence of epistemic uncertainties. However, the number of uncertain factors and plausible scenarios that result from their combined interactions can easily be in the tens or hundreds. The issue was recognized by a recent panel of prospective LCA specialists concluding that "studies with more than three scenarios are outside of the corporate considerations in most situations as the interpretation of results becomes too challenging" (Adrianto et al., 2021). What is often observed in prospective LCA models is that a handful of scenarios are selected that serve as a benchmarking exercise and to identify potential hotspots (Cucurachi et al., 2018; Tsoy et al., 2020). This tendency is also reflected in the European Commission's recently published methodological guideline for the implementation of their SSbD framework (Abbate et al., 2024), which states: "Knowing the product or sector application of the chemical/material under development, it is possible to create scenarios describing the possible variabilities, for instance in terms of geography or products." Given the limited attention span and impracticalities of evaluating hundreds of possible scenarios to make decisions, it is imperative that the relevance of the selected scenarios to safety/sustainability implications is considered before they are selected as a basis for decision-making. This would ensure that potentially important scenarios are not left outside of the analysis. The biases and pitfalls of such ad hoc scenario analysis have been very well discussed by Morgan and Keith (2008).

Global sensitivity analysis (GSA) is an ideal approach to reduce the number of scenarios while taking into account their relevance to the safety and sustainability of the assessed technologies. Rather than testing the sensitivity of a subset of intrinsic and extrinsic factors that are chosen based on pre-established or subjective criteria, GSA allows all uncertain factors in the prospective LCA/risk assessment models to vary freely within their possible ranges, quantifying how their uncertainty contributes to uncertainty in the calculated indicators, both directly and indirectly via interactions with other factors. Through a diversity of methods and approaches, GSA can thus rank uncertain factors in terms of relevance and produce a robust subset of scenarios on which the analysis can be focused (Razavi et al., 2021).

In this paper, we propose a framework that relies on GSA to identify the scenarios of most interest that can result from the different configurations of the most influential factors and use these to prioritize R&D efforts toward SSbD-guided innovation. We developed this framework considering two different types of assessments commonly used to support SSbD: LCA and human health and ecological risk assessment (HERA). An introduction to each is provided by Guinée et al. (2011) and European Chemicals Agency (2011), respectively. The combined use of LCA and HERA is seen as a promising approach for addressing the potential safety/environmental concerns of emerging technologies (Guinée et al., 2017; Kuczenski

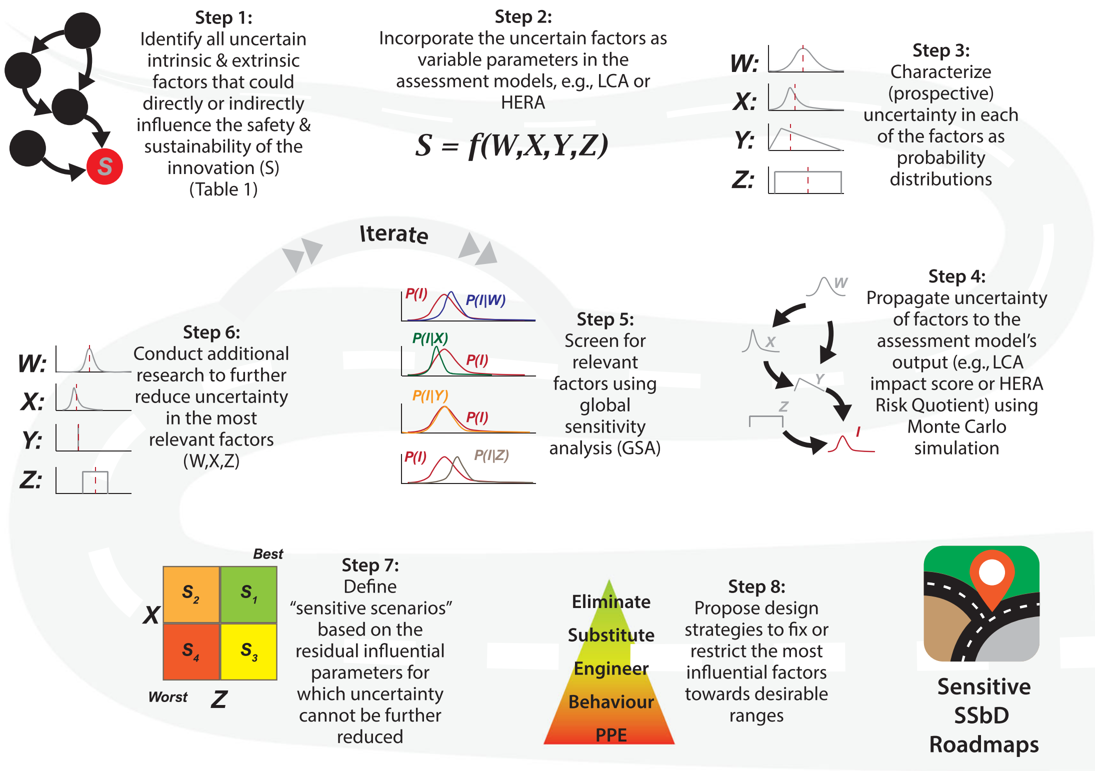

FIGURE 1 Overview of the proposed framework for guiding safe and sustainable-by-design innovation. SSbD, safe and sustainable-by-design; LCA, life cycle assessment.

et al., 2011). Our proposed framework offers a practical way to combine knowledge and insights from the different domains of LCA, HERA, and probability theory in a consistent framework. Particularly, efforts to integrate LCA with HERA have a long history while no clear way forward has emerged yet. Here, we demonstrate how integrating them on the basis of uncertainty and sensitivity analysis can be a very fruitful approach (Cucurachi et al., 2016). Although we focus on these two types of assessments, the framework we propose can be applied to other types of assessments that can be implemented in SSbD frameworks such as social-LCA and life cycle costing. We illustrate the framework with a case study of an emerging PV technology, III-V/Si multijunction cells (Cariou et al., 2018; Essig et al., 2017).

2 | METHODS

2.1 | Framework overview

The framework we propose follows eight steps (see also Figure 1): (i) identifying uncertain factors that could influence safety/sustainability indicators, with special attention to those specific to the forward-looking nature of the assessments; (ii) incorporating these factors as parameters in the models (e.g., prospective LCA or HERA); (iii) characterizing uncertainty in these factors using proposed probability distributions; (iv) propagating the uncertainties using Monte Carlo simulations; (v) screening for relevant factors, by ranking them based on sensitivity using GSA; (vi) conducting additional research to further reduce uncertainty in the most sensitive factors and iterating back to the previous step as needed; (vii) in a final GSA iteration(s), select remaining sensitive factors as a basis to develop relevant scenarios based on sensitivity, which we define as "sensitive scenarios." Sensitive scenarios highlight opportunities for the most effective SSbD improvements for technology designs that are in the early R&D. In a final step (viii) these opportunities for influential design changes are proposed to technology developers as effective roadmaps for SSbD innovation.

2.2 | Identifying uncertain factors

The first step in our framework is to comprehensively screen for and identify uncertain factors in the underlying models, for example, LCA or HERA, which are used to assess safety and sustainability impact/risk indicators. Uncertainty has been comprehensively studied in *ex post* LCA and

HERA models. A practical overview is provided by Lloyd and Ries (2008), who classify uncertainties according to different LCA modeling components: parameter (input data), model (mathematical relationships), and scenario (normative choices). A similar set of uncertainty sources has been described in HERA (U.S. Environmental Protection Agency, 2019). Prospective assessments introduce additional sources of uncertainty due to the forward-looking nature of the assessments. Table 1 extends our previous work (Blanco, Cucurachi, Guinée et al., 2020) as well as that of Miller and Keoleian (2015), proposing a comprehensive typology that can be used to identify these sources of uncertainty, along with relevant examples found in both prospective HERA and LCA models. Rather than the three-group distinction of Miller and Keoleian (2015), we propose a simpler binary distinction between intrinsic/extrinsic, to distinguish factors that are under the direct control of the technology developer and can be directly targeted via design strategies.

It is important to note that there can be overlap or ambiguity between uncertainty types, but this is not problematic as the purpose is to make as comprehensive a screening as possible. For example, uncertainty in a physical constant such as a soil/water partitioning coefficient for a novel substance can be considered either parameter or model uncertainty. Uncertainty in a physical constant can also be classified as scenario uncertainty whereby each scenario represents a future world where the constant has a different value from a range of possible values.

As the aim of this step is to identify and target relevant factors, it is even possible to consider alternative framings, paradigms, and viewpoints as uncertain factors, making the analysis more robust to a broader spectrum of stakeholders and perspectives. For example, the LCA ReCiPe (Huijbregts et al., 2017) impact assessment method's choice between individualist, hierarchist, or egalitarian cultural perspectives (these perspectives determine, e.g., which time horizons should be taken into consideration when quantifying the impacts of emissions: an individualist perspective considers shorter time horizons than an egalitarian perspective).

In the proposed typology of Table 1, we also emphasize the difference between the intrinsic/extrinsic and foreground/background nature of each factor. This difference determines whether design improvements are directly controllable by the technology developer or if indirect design strategies are needed to influence the behavior of other value chain actors.

2.3 | Incorporating uncertain factors as parameters

In the second step, we translate as many uncertainties as possible to a "parameter" type of uncertainty. This requires all potentially influential factors listed in Table 1 to be represented as variable parameters in a *single* integrated LCA or HERA model. This is straightforward for the "parameter" types of uncertainties.

Scenario uncertainties of type I, III, V, and VIII, which are often assessed as separate variations of the model, can also be parametrized within a single model using the approach we demonstrated in previous work (Blanco, Cucurachi, Guinée et al., 2020), where alternative scenarios exist simultaneously in the model and are activated or deactivated stochastically using binomial or multinomial distributions. Model uncertainties—where competing model alternatives exist—can be incorporated similarly, as described by Saltelli et al. (2008) and Mendoza Beltrán et al. (2016).

Some aspects may entail uncertainty that cannot be quantified and translated into parameter uncertainty. We further discuss these types of uncertainties in Section 4.4.

2.4 | Characterizing prospective uncertainty

The third step involves expressing the range of possible values for all factors—including triggers for alternative models and scenarios—as probability distributions. Since we are referring to future events, some precision is warranted as to the interpretation of probability. Two competing interpretations of probability currently dominate the modeling landscape (we discuss other higher-level and broader perspectives in Section 4.4):

- The *frequentist* approach determines probability distributions by conducting numerous tests (or collecting numerous samples) and recording the frequencies of occurrence of each value. Such tests or samples can only be collected once a technology is deployed. This approach is evidently of limited use in prospective assessments.
- The *Bayesian* approach uses probability distributions to represent a degree-of-belief or plausibility: how much we think that something is true, based on the evidence at hand (Jaynes, 2003; Sivia, 2006). The Bayesian approach has been applied in risk assessment (Smith & Kelly, 2006) and to a lesser extent in LCA (Lo et al., 2005; Miller et al., 2013). It is especially useful for prospective assessments, if not essential, given that many factors cannot be observed and randomly sampled as required by the frequentist approach.

While frequentists have long argued that subjectivity is a weak point of Bayesian analysis (or outright precluding its scientific validity), it is also a key strength in that it incorporates other sources of relevant information and expert knowledge where actual observation data are scant or unavailable. Bayesians also argue that subjectivity is pervasive, yet it is less transparent in the frequentist approach (Sivia, 2006)—and, in our view, even

TABLE 1 Uncertain factors in prospective safe and sustainable-by-design (SSbD) assessments of emerging technologies.

Domain	Type	Intrinsic (I)/Extrinsic (E)	Uncertain factor	Uncertainty type	Miller and Keoleian classification	LCA model component	HERA model component	Context and examples
Technology design	I	I	Material choice	Scenario	Not covered	Inventory (foreground)	Similarity estimates	Different materials will be tested and selected based on optimized performance; more recently safety, chemical simplicity, and recyclability are also considered. See Blanco et al. (2020) (metallization of PV cells).
	II	I	Material quantity	Parameter	Not covered	Inventory (foreground)	Emission scenario	Quantities of materials incorporated in the final product design may vary as the design gets optimized for volume/weight/form/etc. See Cucurachi et al. (2021) (silicon PV cells).
Technology manufactur-ing	III	I	Manufacturing route	Scenario	Not covered	Inventory (foreground)	Emission scenario	Manufacturing/synthesis methods may change when upscaling to an industrial scale. See Piccinno et al. (2016) (chemicals).
	IV	I	Material and energy use	Parameter	Not covered	Inventory (foreground)	Emission scenario	Process optimizations likely lead to reduced material and energy consumption. See Cucurachi et al. (2021) (silicon PV cells).
Technology supply chain	V	E	External suppliers' processes	Scenario	Supply chain/exogenous system effects	Inventory (background)	Emission scenario	Analogous to (III) but applied to external suppliers.
	VI	E	External suppliers' materials & energy use	Parameter	Supply chain/exogenous system effects	Inventory (background)	Emission scenario	Analogous to (IV) but applied to external suppliers. See Harpprecht et al. (2021) (metals).
	VII	E	Functional performance of suppliers' processes	Parameter	Supply chain/exogenous system effects	Inventory (background)	N/A	Background processes/ancillary services may be optimized for better performance, for example, increased recycling or abatement efficiencies by third-party waste handlers.
	VIII	E	External markets composition	Scenario	Supply chain/exogenous system/spatial effects	Inventory (background)	Emission scenario	Changes in market compositions for products and services in the supply chain. See Mendoza Beltran et al. (2020) (energy) and Harpprecht et al. (2021) (metals).
	IX	E	Allocation	Model	Exogenous system effects	Inventory (foreground)	N/A	The parameters used to establish the criteria for the allocation of multifunctional processes may change over time, for example, forecasted market values in the case of economic allocation in LCA.

(Continues)

TABLE 1 (Continued)

Domain	Type	Intrinsic (I)/Extrinsic (E)	Uncertain factor	Uncertainty type	Miller and Keoleian classification	LCA model component	HERA model component	Context and examples
Technology use	X	I/E	Function of technology	Scenario	Efficiency and functionality change/rebound effects/behavior change	Goal and scope	Emission scenario	The technology may ultimately be used in different ways. It may be used more or less than expected and/or for multiple/different purposes. See Hiremath et al. (2015) (batteries) and Hischier et al. (2017) (engineered nanomaterials).
	XI	I/E	Survival/failure rates	Parameter	Efficiency and functionality change	Inventory (foreground)	Emission scenario	Failures (due to, e.g., obsolescence, degradation, or misuse) may cut the technological products' lifetimes short. See Miller and Keoleian (2015) (online commerce).
	XII	I	Functional performance	Parameter	Efficiency and functionality change	Goal and scope	Emission scenario	The technology's operational performance parameters may deviate from expected values. See Gong et al. (2015) (perovskite PV).
Technology EoL	XIII	I/E	Recycling	Parameter/ scenario	Resource criticality	Inventory (foreground)	Emission scenario	The development of recycling methods often *lags behind* technology deployment. It is not known whether and how this will happen. See Raugei and Winfield (2019) (battery recycling).
Regulatory	XIV	E	Material use and emission thresholds	Parameter/sce	Policy and regulatory effects	Inventory (background)	Emission scenario	Regulation may impose new limits on emissions, use, or choice of materials and energy sources.
Environment/ Landscape	XV	E	Characterization model: fate	Parameter	Not covered	Impact assessment	Fate	Landscape parameters that may affect the transport and fate of the substances can change in time, for example, changing averages for ambient temperatures, wind speeds, or ocean water pH can affect how substances are distributed in the environment.
	XVI	E	Characterization model: exposure	Parameter	Not covered	Impact assessment	Exposure	Parameters that affect exposure, for example, population densities or diets can change in time.
	XVII	E	Characterization model: effect	Model	Not covered	Impact assessment	Effect	Marginal changes may result in exponentially larger effects as the baseline condition deteriorates, for example, the impact of increased radiative forcing on ecosystems.
	XVIII	E	Resources	Model	Resource criticality	Impact assessment	N/A	Availability of natural resources may change over time. This can particularly affect LCA impact categories related to resource depletion. See Baustert et al. (2022) (water scarcity).

Note: Factors are classified according to their modeling domain and whether they are extrinsic or intrinsic to decision-making during the R&D process. Expands on Miller and Keoleian (2015) and Blanco, Cucurachi, Guinée et al. (2020).
Abbreviations: EoL, end-of-life; LCA, life cycle assessment; PV, photovoltaic.

more so in prospective assessments. Nevertheless, Bayes' theorem obeys the rules of probability and provides a formal method for updating the initial beliefs (represented by so-called *prior* probability distributions) with new data that become available to produce a *posterior* distribution (Sivia, 2006). As a simple example, we may hold a prior belief that a novel solar PV cell design will have a conversion efficiency between 30% and 35% (following Table 1, this is a type XII factor which we could model as a uniformly distributed variable with min = 0.30 and max = 0.35). If a series of pilot tests during R&D exceed expectations and demonstrate efficiencies up to 36%, then we need to update our priors to be consistent with these new data. It is important to highlight that for the modeler, 36% will not be the final (true) value; the PV cell's conversion efficiency will remain uncertain and may be reduced or increased again depending on the evolution of the technology design, which will be subject to numerous other factors. However, our updated prior is that efficiency will more likely be in a higher range. This iterative process of updating priors naturally fits the R&D process, which subjects a technological concept to extensive testing and gradual upscaling to optimize it until it is ready for commercialization.

Adopting a Bayesian perspective, the question then is how best to establish prior distributions for uncertainties of the types listed in Table 1, and then how to update them. A conservative (as in *less subjective*) attempt could be to start with relatively flat or so-called "uninformative" priors, which distribute probabilities almost evenly across all possible parameter values. We note, however, that "uninformative" is a misnomer, since any prior will convey some information. Detailed discussion on the strengths and limitations and guidance for choosing priors can be found in Gelman et al. (2013). However, this approach comes with a trade-off on how informative subsequent posteriors will be. Wolpert et al. (1993) discuss this situation and offer that—with important caveats and limitations—"collateral evidence" such as that obtained from field studies of similar environmental systems, expert elicitation, and laboratory studies of the related process can be used to inform priors. Another often-applied rule of thumb in Bayesian statistics is to choose priors from a "conjugate distribution family." Conjugate priors ensure that the functional form of the resultant posterior distribution is the same as that of the prior; that is, a normal prior probability density function will be updated to a normal posterior probability density function (Gelman et al., 2013). Conjugate priors can also make the estimation of posterior distributions a simpler and more intuitive exercise once additional data or observations are obtained.

Before moving to the next step, we take a small side note to mention a potential role for the well-known *pedigree* approach that has been widely applied in LCA (Muller et al., 2014). The pedigree approach is based on the NUSAP principles for management and communication of uncertainty in science for policy (van der Sluijs et al., 2005). The pedigree approach proposes semiquantitative indicators of data quality, based on aspects such as temporal/geographical/technological representativeness. In the widely used *ecoinvent* database (Wernet et al., 2016), the data quality indicators are then used to derive (pseudo) uncertainty distributions based on rules of thumb. In our framework, we purposely refrain from propagating this *pedigree* (pseudo) uncertainty due to its semiquantitative nature. However, the pedigree approach can help pinpoint potentially influential factors with a low pedigree in the background systems (supply chains) that may especially deserve inclusion in the analysis.

2.5 | Propagating uncertainty

Once the uncertainty in influential factors has been characterized, we must analyze how it reflects on the models' outputs, that is, LCA or risk assessment indicator scores. Two approaches for propagating uncertainties are commonly applied: analytic and numerical (Groen et al., 2014). The models' complexity and the fact that integrated assessments require interaction between different types of models make analytical solutions impractical for this type of framework. The more convenient alternative is Monte Carlo simulation (Firestone et al., 1997), which simulates numerous random samples from the underlying probability distribution of the model's input parameters and calculates an equal number of values for the model's output, for example, an LCA impact score or risk quotient. The results of the uncertainty propagation via Monte Carlo are directly used in the next step to conduct the GSA.

2.6 | Screening for relevant factors

GSA reveals "how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input" (Saltelli et al., 2008). In our framework, GSA is used as the sieve which selects the most relevant factors from all those identified. The characteristics of the integrated models we use place certain constraints on the type of GSA that can be performed. First, it is likely that the resulting models will be highly dimensional with numerous uncertain parameters. This requires sensitivity calculation algorithms that can be performed in a reasonable computational time. Second, the models are usually integrated by passing output data as input data between them (as in the integration of economic demand with emissions and fate models), which makes analytical GSA methods less practicable if a closed-form mathematical representation and solution for the integrated model is not available. "Black box" or model-independent GSA methods are thus favored. Third, the introduction of binomial and other discrete distributions for factors could result in multimodal output distributions for LCA or risk scores (Blanco, Cucurachi, Guinée et al., 2020). Therefore, variance-based methods may not be suitable, and moment-independent methods are preferred (Borgonovo, 2007; Borgonovo & Iooss, 2017).

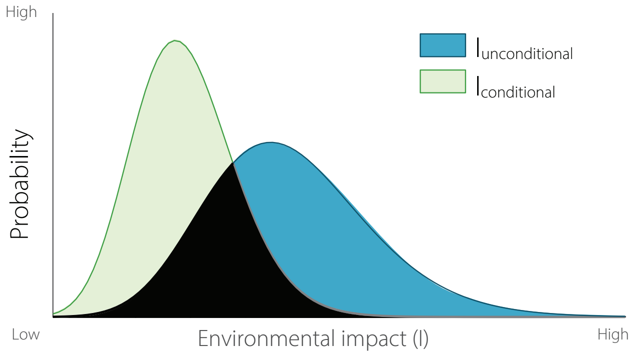

FIGURE 2 Graphical representation of the "shift" in a distribution curve, used to calculate Borgonovo's delta sensitivity measure in an environmental model. The non-overlapping area (non-black) represents the shift in the curve when the model is evaluated conditional to an uncertain factor fixed at one of its possible values. Adapted from Borgonovo (2007).

As we demonstrated in previous work (Blanco, Cucurachi, Guinée et al., 2020; Cucurachi et al., 2021), one GSA method that meets these requirements is the *delta* sensitivity measure proposed by Borgonovo (2007). The Borgonovo *delta* defines the influence of a parameter as its ability to shift the model's output distribution curve. This is illustrated by Figure 1, where the blue probability distribution curve is the environmental risk of a technology when all uncertain factors are left to vary freely across their entire spectrum of possibilities, according to their underlying distributions ($I_{unconditional}$). If one factor in the risk model can be fixed at a value representing one scenario, the curve will shift by moving along the *x*-axis (lower or higher risk depending on the state of the factor) and will become narrower (lower uncertainty/dispersion in the model output or risk score). The new green curve ($I_{conditional}$) is the probability distribution of the environmental risk for the specified scenario. For an LCA/HERA indicator, two things are desirable: that the output distribution curve moves toward the origin on the *x*-axis (lower risk/impact) and becomes narrower (less uncertainty). The curve's *shift* is defined by Borgonovo as the non-overlapping area between both curves (red plus blue and not purple). The *delta* sensitivity measure is the probability-weighted average of all shifts induced by the uncertain factor when it is fixed at its possible values (Borgonovo, 2007).

2.7 | Further reducing uncertainty

The first GSA iteration may result in several factors that have higher sensitivity, that is, are more influential. Before producing recommendations or making any decisions on the technology design, three recourses can be used to further reduce uncertainty in the most influential factors. First, subjective probability estimates can be refined by structured expert knowledge elicitation protocols, which are aimed at reducing bias while furthering consensus (Hanea et al., 2018; Morgan, 2014; Wang et al., 2012). Some of these methods have already been extended to incorporate the experts' beliefs regarding their own uncertainty about their estimates (Wang et al., 2012). Second, more refined modeling can be applied depending on the nature of the parameter, for example, hydrological, geochemical, process simulation, or economic models. A third recourse is to collect additional data from lab or pilot-scale tests, such as leaching tests or emissions measurements. As explained in Section 2.3, Bayesian inference can be used to update the prior probability distributions for the factors for which new data were obtained. An additional strategy that has been proposed recently to fill data gaps in LCA of emerging technologies is the use of predictive machine learning algorithms (Romeiko et al., 2024). However, these may not necessarily reduce uncertainty and on the other hand, introduce other sources of uncertainty (due to model error/approximations), which should be taken into account as well.

2.8 | Defining sensitive scenarios

Once the possibilities to further reduce uncertainty have been exhausted, additional uncertainty propagation and GSA iteration will produce the residual influential factors. These factors can then be used to construct "sensitive scenarios," which will analyze a smaller, but highly relevant subset of factors. Sensitive scenarios can be used to engage with technology developers and other stakeholders (e.g., suppliers, consumers, policymakers, funding agencies, and environmental advocacy groups) around the prioritization of design strategies that can most effectively lead to safer and more sustainable deployment of the technology. In other words, sensitive scenarios point to the factors that are most influential *while potentially subject to change*. This presents an opportunity to influence these factors by attempting to fix them in the design at a desirable value or at least reduce their uncertainty toward a smaller and more desirable range (shift the risk or impact score distribution illustrated in Figure 2 to the left and make it narrower).

2.9 | Proposing effective SSbD innovation roadmaps

Because sensitive factors can span different domains, their nature may vary significantly as will the possible ways to influence them. A well-tested guiding principle that has been applied for decades in occupational health and safety risk management is the hierarchy of risk control measures, which leads the decision-maker to prioritize risk mitigation strategies according to the order (i) elimination, (ii) substitution, (iii) engineering control, (iv) behavioral controls, and (v) personal protective equipment. Such strategies are already very visible in, for example, proposals for emerging PV technologies, such as in situ sequestration of lead in perovskite solar cells (Li et al., 2020) (engineering control) and replacement of lead (substitution) (Cao & Yan, 2021; Serrano-Lujan et al., 2015). From the technology developer or designer's viewpoint, strategies along the first three tiers of the hierarchy may be easy/intuitive to implement, for example, substituting a chemical, reducing the size of the product, etc. However, when strategies in these tiers have been exhausted, the fourth tier can offer important additional opportunities to influence consumer behavior by modifying the product's design. A very valuable guide for this can be found in Bhamra et al. (2011). Additional ecodesign principles and strategies have been listed in the European Commission's SSbD framework (Caldeira et al., 2022). The most feasible and effective strategies found in this step would form the basis for highly effective SSbD improvement roadmaps.

3 | CASE STUDY: MULTIJUNCTION III-V/SILICON PHOTOVOLTAICS

3.1 | Case study description

To illustrate the proposed framework, we apply it to an emerging PV technology, high-efficiency III-V/silicon multijunction cells. In previous work, we conducted a comprehensive LCA (Blanco, Cucurachi, Dimroth et al., 2020) and an ecological risk assessment (Blanco et al., 2024) of this technology. These assessments were primarily based on data obtained from laboratory-scale and pilot studies conducted within a European R&D project (Fraunhofer ISE, n.d.). In the following sections, we will explain how these models and insights about the technology evolved by applying the framework (in some aspects, retrospectively). We will consider three iterations of the LCA and RA models, which correspond to different stages: the state of knowledge at an early stage of the R&D project (*t*0), after addressing key uncertainties through the project's R&D efforts (*t*1), and an optimized roadmap achievable by fixing residual sensitive factors at optimal values (*t*2). We summarize how the framework is applied step-by-step in Table S1 of the Supporting Information file S1 and explain the most relevant aspects in the following sections.

3.2 | Life cycle assessment

The manufacturing of III-V/Si cells involves numerous processing steps, most of which are already deployed at an industrial scale in the mainstream silicon PV industry. Two key steps, however, are early-stage concepts that could only be tested at lab and pilot-scale and thus brought about large uncertainties. The first is the deposition of the top cell's III-V layers, which are grown via metalorganic vapor phase epitaxy (MOVPE; Dimroth, 2017). In the initial phase of the project (*t*0), we considered commercial MOVPE reactors that are widely used in PV and related industries. Early experimental runs conducted during the project showed these reactors to have a high energy consumption with low throughputs (7 round 4″ wafers per run at 3.5-h runtime). The second is the metallization of the cell's front contacts, for which a choice had to be made between highly experimental nanosilver and nano-copper ink and their corresponding synthesis and sintering routes, as described in previous work (Blanco, Cucurachi, Guinée et al., 2020).

A third uncertain aspect was the final performance that could be achieved by the III-V/Si PV panels (in terms of energy yield) since a final design was not available for testing. The same applies to panel lifetime, which also depends on consumers not replacing them before the end of their useful life. These performance uncertainties are reflected in the model in three factors: panel efficiency, performance ratio, and panel lifetime. Additional uncertainties existed in the background silicon supply chains and other PV components, which are described in Cucurachi et al. (2021). The initial state of knowledge for all identified uncertain factors at this early stage of the project was represented with the probability distributions shown in Table 2, *t*0.

Propagating all uncertainties at *t*0 resulted in a wide distribution, with climate change impact score ranging between 0.03 and 0.74 kg CO_2eq (Figure 3, *t*0). A GSA for this first iteration highlighted the sensitivity importance of the power consumption of the MOVPE tool (*P_movpe_tool*), followed by MOVPE runtime (*RT_movpe*) and panel lifetime (LT_panel) (Figure 4, *t*0). A second tier of influential factors was found in the background silicon supply chain as well as the choice between copper and silver nanoink (*Cu_vs_Ag*) for the front metallization and the chances of success of the different nanoparticle synthesis and ink sintering routes (*p*1–*p*5). In the case of binomially distributed factors, the underlying probabilities p_x of each were more influential than the factors themselves.

TABLE 2 Evolution of uncertain factors in a life cycle assessment (LCA) model of the III-V/Si tandem photovoltaic technology.

Factor Id	Factor description	Uncertainty type (from Table 1)	First iteration ($t0$)	Second iteration ($t1$)	Final iteration ($t2$)
MOVPE					
P_movpe	MOVPE tool power load per processed wafer area	IV	pert(min = 1, mode = 509, max = 509)	pert(min = 1, mode = 119, max = 119)	15
RT_movpe	MOVPE runtime	IV	pert(min = 0.5, mode = 3.6, max = 3.6)	pert(min = 0.5, mode = 2.6, max = 2.6)	0.5
Scru_cons	Scrubber granulate consumption	IV	triang(min = 2.55, mode = 7.65, max = 7.65)	No change	No change
Front metal*					
Cu_v_Ag	Choice of Cu nanoink versus Ag nanoink	I	bin(1, p_1) $p_1 \sim$ beta(4,2)	bin(1, p_1) $p_1 \sim$ beta(7,3)	1 (resolved for copper nanoink)
Synth_Ag	Choice of chemical versus physical synthesis for Ag nanoink	V	bin(1, p_2) $p_2 \sim$ pert(1000, 0.5,0.7,0.8)	No change	Not applicable
Synth_Cu	Choice of chemical versus physical synthesis for Cu nanoink	V	bin(1, p_3) $p_3 \sim$ pert(1000, 0.5,0.7,0.8)	No change	No change
Sint_Cu	Choice of laser versus chemical sintering for Cu nanoink	III	bin(1, p_4); $p_4 \sim$ pert(min = 0.1, mode = 0.2, max = 0.3)	1 (resolved for laser sintering)	No change
Sint_Ag	Choice of laser versus. chemical sintering for Ag nanoink	III	bin(1, p_5); $p_5 \sim$ unif(1000, 0,1)	No change	Not applicable
Performance parameters					
Eff_panel	Panel efficiency	XII	pert(min = 0.25, mode = 0.28, max = 0.31)	No change	0.31
PR_syst	Performance ratio of PV system	XII	pert(min = 0.8, mode = 0.85, max = 0.9)	No change	No change
LT_panel	Panel lifetime	XI	norm(30, 5)	No change	35
Background supply chain					
Cu_scrub	Scrubber granulate copper fraction	VI	pert(min = 0.2, mode = 0.3, max = 0.7)	No change	No change
Cu_rec	Recycling of copper from granulate	V	bin(n = 1, p = 0.5)	No change	No change
Al_panel	Aluminum in panel	II	lnorm(gm = 2.63, gsd = 1)	unif(1000, min = 1.6, max = 2)	No change
Glass_panel	Glass in panel	II	lnorm(gm = 10.08, gsd = 1.22)	unif(1000, min = 5.04, max = 7.56)	No change
Elec_panel	Electricity to manufacture panel	IV	lnorm(gm = 4.71, gsd = 1)	unif(1000, min = 12.22, max = 15.27)	No change
Elec_siem	Electricity consumption Siemens process	VI	lnorm(gm = 110, gsd = 1)	unif(1000, min = 34.1, max = 44.3)	No change
Heat_siem	Heat consumption Siemens process	VI	lnorm(gm = 185, gsd = 1)	unif(1000, min = 57.24, max = 74.52)	No change
Elec_CZ	Electricity consumption Czochralski process	VI	lnorm(gm = 85.6, gsd = 1.22)	unif(1000, min = 43.4, max = 69.3)	No change
Si_CZ	Silicon consumption for Czochralski process	VI	lnorm(gm = 1.07, gsd = 1)	triang(1000, min = 0.4, mode = 0.66, max = 0.75)	No change

*For the front metal components, the five uncertain choices are represented by two uncertain factors each: the choice (a variable equal to 1 or 0) and the chances of success for the given choice, which is represented by an uncertain factor p_x. The initial model then has 25 uncertain factors in total.
Abbreviations: MOVPE, metalorganic vapor phase epitaxy; PV, photovoltaic.

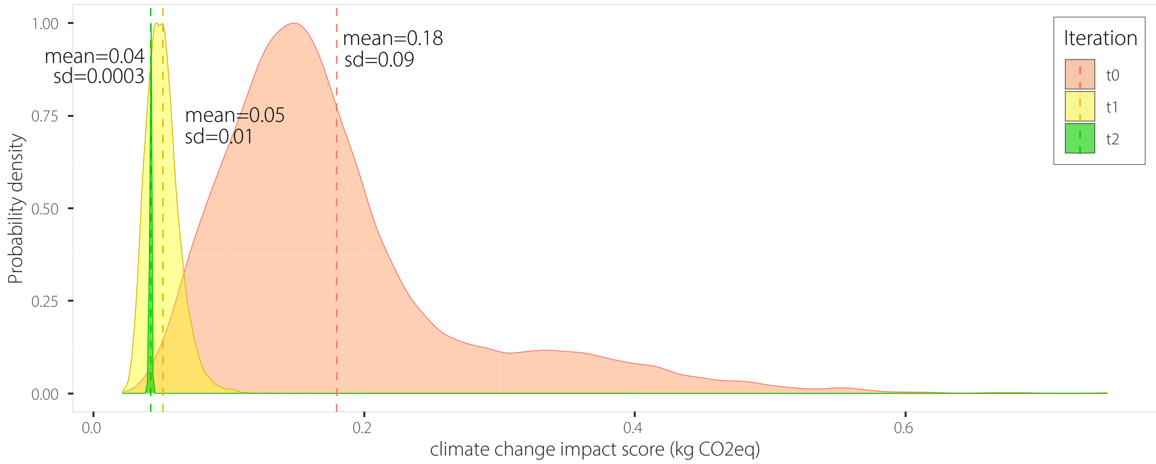

FIGURE 3 Probability distribution for climate change impact scores of the emerging III-V/Si technology in three successive iterations: *t*0 = early stage of research and development (R&D) project, *t*1 = after R&D project, and *t*2 = optimized roadmap for the technology.

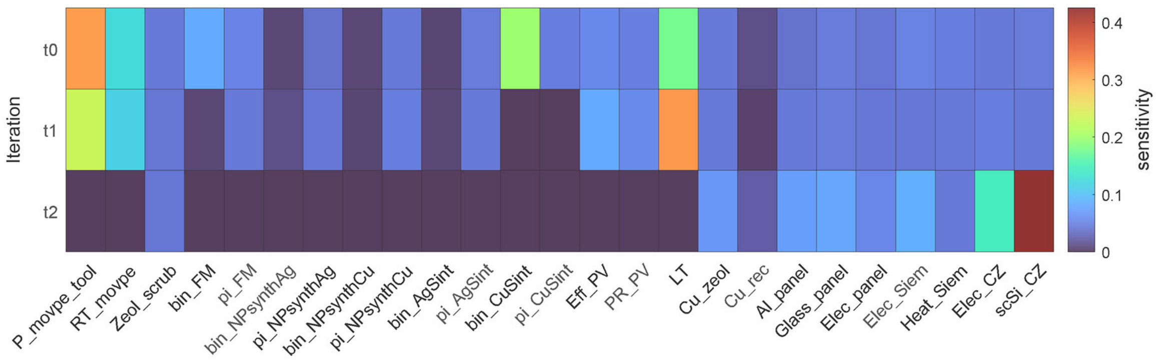

FIGURE 4 *delta* sensitivity measures (relative to other factors) in three successive iterations: *t*0 = early stage of the research and development (R&D) project, *t*1 = after R&D project, and *t*2 = optimized roadmap for a market-ready technology. The description of each factor is provided in Table 2.

MOVPE reactor optimization was a clear R&D priority and by the end of the project (*t*1), a pilot-scale reactor achieved a throughput of 31 round 4-in. wafers per run at 2.5 h runtime. Additional research and testing were conducted on the metallization as well, showing more promising results for copper, while the LCA flagged the chemical sintering route as an environmental hotspot. We thus applied Bayesian updating of the binomial distributions representing the chances of copper and laser sintering being preferred. Some additional factors in the background silicon supply chain and other non-cell components were also updated in *t*1 to better reflect state-of-the-art as reported in the earlier publication by Cucurachi et al. (2021).

At the end of the R&D project (*t*1), the expected (mean) climate change impact score was greatly reduced, as well as the uncertainty around it (Figure 3, *t*1). The influence of MOVPE power consumption was also reduced and the most sensitive factor by a considerable margin was the panel's lifetime (Figure 4, *t*1). This presents an interesting opportunity; III-V cells on germanium rather than silicon substrates have been designed in the past to withstand extreme radiation for their applications in space, so there may be a good case for III-V/Si cells to last longer than conventional silicon ones. Following the hierarchy of risk controls suggested in Section 2.9, this would constitute a very effective engineering control. In addition to this, the high efficiency of III-V/Si cells means that they are less likely to become obsolete before they reach their EoL.

The project also concluded that an even larger reactor throughput would be required to make the technology economically and environmentally competitive. Possibilities to further increase MOVPE throughput and reduce runtime were elicited from experts, based on what they would consider feasible future developments in MOVPE reactor design. Such improvements include switching to larger wafers (square M2-type wafers) and increasing throughput to 50 wafers per run at 0.5 h runtime. A "sensitive" roadmap for SSbD optimization would thus continue to pursue copper laser-sintered metallic front contacts while targeting best-case values for MOVPE power consumption and runtime and panel efficiency, and taking action to increase the durability of the panel while putting in place administrative controls to avoid early obsolescence/discarding by consumers. Such an optimized roadmap (*t*2) could lead toward a reduction in the mean impact score from 0.05 to 0.04 kg CO_2eq, with a very low standard deviation of 0.0003 (Figure 3, *t*2).

TABLE 3 Evolution of key factors in the ecological risk assessment model of the III-V/Si tandem photovoltaic technology.

Factor description	Uncertainty type (from Table 1)	First iteration (*t*0)	Second iteration (*t*1)	Final iteration (*t*2)
PV capacity demand	No uncertainty modeled	Steady-state 5 GW capacity addition per year.	Dynamic, logistic growth curve based on >1000 datapoints.	No change
Arsenic waste leaching in landfill	XV	Constant rate (% mass/year). Empirical, based on two datapoints; a lognormal distribution was assumed with a mean of 0.8 and variance if 0.3.	Dynamic, calculated from (uncertain) solid/waste partitioning coefficient (k_{sw}) uncertainty estimated from >100 datapoints (Allison & Allison, 2005).	Leachate pH controlled resulting in higher k_{sw} (now sampled only from the upper quartile of the distribution used in t1).
Leakage of landfill leachate to surrounding soil compartment	XV	Constant leakage rate of landfill leachate to the surrounding soil compartment (%/year): based on 1 datum, a lognormal distribution was assumed with a mean of 2.0 and variance of 0.7.	Uncertainty estimated from landfill infiltration rates based on >100 datapoints (U.S. Environmental Protection Agency Office of Solid Waste, 2003).	No change.
Landfill cell depth	XV	Not applicable.	Empirical, exponential distribution with a peak at 10 and lower value of 0.5 m based on >100 datapoints (U.S. Environmental Protection Agency Office of Solid Waste, 2003).	Increased landfill depths (PERT distribution with min = 5, mode = 7.5 max = 10 m).
Recycling rate	XIII	Uniform distribution assumed for 85%–99.9% of panels collected.	No change.	Shifted to 95%–99.9% panels collected.
Incinerator abatement	VII	Uniform distribution assumed for 98%–99.9% arsenic captured in an electrostatic precipitator.	No change.	Shifted to 99.5%–99.9% arsenic captured in the electrostatic precipitator.
Fate parameters in the SimpleBox fate model	XV	No uncertainty modeled.	Uncertainty estimates based on Bakker et al. (2003).	No change.

Abbreviation: PV, photovoltaic.

3.3 | Risk assessment

A first iteration of an ecological risk assessment for the III-V/Si PV technology (*t*0) was conducted during the early stages of the R&D project, based on a highly simplified and conservative model (Blanco, Cucurachi, Peijnenburg et al., 2020). A prospective risk quotient (RQ, also *risk characterization ratio* [*RCR*] as described in European Chemicals Agency, 2016) was calculated as a ratio of predicted environmental concentrations to predicted no-effect concentrations for arsenic, gallium, and indium emissions from the III-V/Si panels. Table 3 (*t*0) summarizes the key assumptions and uncertain factors that were considered in this simplified model. The distribution of the risk quotient obtained for arsenic emissions to soil in a no-recycling scenario (no arsenic recovered from PV panels collected for disposal) had a mean value of 0.136 (where the threshold for concern is 1) and a small relative standard deviation of 9.06×10^{-3} (Figure 5, *t*0).

A global sensitivity analysis of this first iteration highlighted the leaking rate and the leaching rate as the most sensitive parameters. Thus, increased focus was placed on the landfill emissions component of the model during the remainder of the R&D program. The model was refined in a second iteration (*t*1) as presented in Blanco et al. (2024) with leaching processes reparametrized in terms of a solid/waste partitioning coefficient (k_{sw}) for which more than 100 data points were available. Leakage processes were also reparametrized in terms of landfill infiltration, for which more than 100 data points were available. Additional uncertainty information that became available was introduced in the fate model parameters (which were fixed in *t*0), resulting in over 100 uncertain parameters with uncertainty distributions taken from the literature. For brevity, these are not reported in Table 3, but we refer the reader to Blanco et al. (2024) for a full documentation of the refined model.

Furthermore, in the refined model of *t*1, arsenic emission and fate processes—along with the projected growth in III-V/Si PV demand—were modeled dynamically rather than steady-state, recognizing the relevance of the temporal dimension and reflecting more realistic scenarios (Table 3, *t*1). The resulting risk quotient for arsenic in the soil compartment in Europe in the 100th year of the simulation period was negligible (Figure 5, *t*1). It is the case that the model used in *t*0 has a different scope (steady-state) than the one in *t*1 (dynamic), thus the observed difference in the calculated

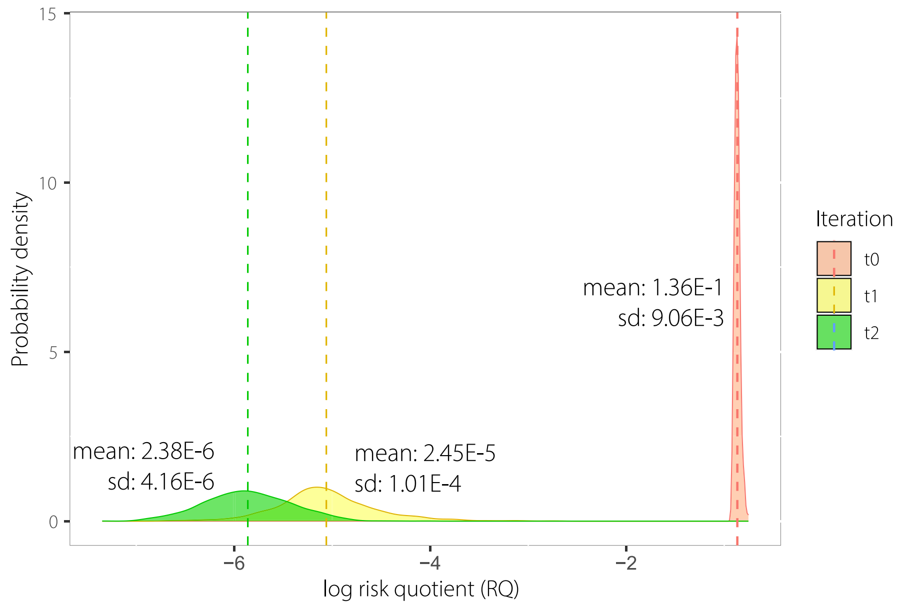

FIGURE 5 Probability distribution of risk quotient for III-V/Si arsenic emissions to the soil in the European continent in three successive iterations: *t*0 = early stage of the research and development (R&D) project, *t*1 = after R&D project, and *t*2 = optimized roadmap for the technology. The description of each factor is provided in Table 3. sd, standard deviation.

risk quotients. Although in *t*0 the risk quotient is calculated in a fundamentally different situation than *t*1, we present the results side by side to illustrate how the problem framing and model choice/setup can also be substantially revised as a result of identifying aspects with large uncertainty and influence. This also shows that GSA can successfully pick problematic areas in the model framing, a key application of GSA referred to in the literature as "sensitivity auditing" (Saltelli et al., 2021).

Here we also note that in refining the model, the relative standard deviation (standard deviation relative to the mean) increased rather than decreased between *t*0 and *t*1. We do not see this as a setback in the implementation of the framework, but rather as an increase in model accuracy at the expense of precision. This can be desirable, especially for long-term forecasts. For a detailed discussion of this important distinction in the context of LCA, we refer the reader to Heijungs (2020).

The GSA in iteration *t*1, pointed to four factors to prioritize for improvement strategies: the waste/leachate partitioning in the landfill, the landfill depth, the recycling rate, and the incinerator abatement. The combined effect of design strategies and improvements targeting these factors (see Blanco et al., 2024) can be evaluated in an "optimistic" future scenario *t*2, where the risk and the relative standard deviation could be reduced by an additional order of magnitude (Figure 5, *t*2).

4 | DISCUSSION

4.1 | Insights obtainable through the framework

Applying our framework to the LCA of the III-V/Si PV system highlighted an interesting point regarding the lifetime of PV panels. While it is common in LCAs of PV to standardize the lifetime parameter to a fixed value, for example, 25 or 30 years (Frischknecht et al., 2016), there is an important variability coming from two different sources. On one hand, there is the stability of the cell/panel and its ability to withstand weathering and degrade slowly. Some opportunities for improvement in this sense lie within the grasp of the technology developer. III-V/Si cells already present an important advantage as they can withstand high radiation for long periods of time without degrading. Further work on improved cell coatings and panel glass framing may offer important roadmaps for more sustainable design. On the other hand, there is the proper maintenance and protection of the panel during its use phase and—perhaps more importantly—the commitment to use the panel throughout its entire useful life and not replace it earlier than needed. The latter opportunities are on the side of the consumer. Our analysis indicates that if the technology developer undertakes all foreseeable actions to improve the manufacturing and design, then the influence the consumer has over the panel reaching its EoL too early will significantly outweigh additional marginal improvements that can be achieved on the design side. Furthermore, we note that the performance ratio (PR_syst), which can also be influenced by the user via adequate maintenance/cleaning and proper installation setup, had a moderate ranking in sensitivity (Figure 4). In a way, these recommendations follow the progression of the hierarchy of risk controls, where engineering controls (design changes) are exhausted and behavioral controls follow next.

In the same way, the risk assessment offered interesting insights that would have been hard to obtain without such a systematic approach to uncertainty. For example, the ethyl vinyl acetate (EVA) layer encapsulating PV cells can dissolve, increasing acidic conditions in landfills and triggering arsenic release. Knowing the importance of this effect gives another reason to reconsider using EVA, which also complicates PV recycling. We refer the reader to Blanco et al. (2024) for further insights obtained in the risk assessment study.

4.2 | Feasibility and resources required

One concern is whether applying all the steps of the framework is possible considering the time and resources typically allocated to such assessments. Fortunately, despite there being a large theoretical work underpinning each step of the framework, the tools for implementation have been developed over time and can now be run in matters of minutes with average computational power (Cucurachi et al., 2021). Compared to the effort typically invested in conventional ex post assessments, the only step that may require significant additional time and data collection is the characterization of uncertainty with probability distributions. In practice, many information exchanges will and should take place between an LCA/HERA modeler and a technology developer. Framing these exchanges in the context of uncertainty as we have presented here will provide more structure to the conversations and optimize the learning process (for both the modeler and the technology developer, as we have often observed in practice).

Furthermore, the most time-consuming refinement is expected to happen during the additional iterations to reduce uncertainty, which will—after GSA—only consider a handful of uncertain factors in the model. The alternatives to our proposed approach could be equally or more time-consuming, for example, developing and communicating numerous ad hoc scenarios or developing more detailed modeling such as process engineering upscaling for uncertain parameters. Our framework can reduce the R&D resources spent trying to optimize non-influential parameters and ensures that the additional resources required are spent on the things that matter.

4.3 | On subjective probability distributions

Another concern is whether it is realistic, robust, and transparent to introduce largely subjective probability distributions that may obfuscate the underlying models' assumptions and their results. Here, we argue that exactly the opposite is the case; the subjective assumptions are not only clearly stated but they are represented in a way that obeys the rules of probability. The effects of these assumptions are systematically introduced, analyzed, and interpreted. Two types of assumptions are required in our framework when subjective distributions are used. First, the shape of the distributions (e.g., uniform, PERT, triangular), and second, the parameters of the distribution (e.g., min, max, and mode). The case study offers a good example of how we introduced boundaries and realistic assumptions in the energy consumption of the MOVPE process. We chose a PERT distribution bounded by the maximum power loading, which is given by the best result achieved to date. This is reasonable as it was already established that the current consumption is not economically viable. The minimum is a very low value that resembles that of in-line tools used in the high-throughput production of commercial silicon cells, which have 30 or more years of advantage. For a conservative approach, we set the mode equal to the maximum. We could have chosen a triangular shape using these minimum and maximum boundaries. However, a PERT shape is more realistic in that increases in energy efficiency get more difficult with each subsequent attempt.

This example shows how relevant and objective information that would be lost otherwise is included in the distribution. On the other hand, making no assumption is in many ways an assumption. For example, not attaching probability to different scenarios may well result in the unconscious attachment of equal probability to each scenario during the interpretation and/or decision-making phase. Interpretation and decision-making will necessarily involve probabilistic weighing, whether it is done by the modeler or the decision-maker, consciously or unconsciously. Given the rigor introduced here, we advocate it is best to place probabilistic weighing as much as possible within the scope of the assessment itself. In addition to this, it must be recognized that prospective assessments are inevitably conducted in low-information environments. Therefore, all information available should be used, including beliefs, constraints, and possible states that narrow the space for ambiguity. As a final note, we highlight that the choice of probability distributions is an (uncertain) modeling element that can be tested within the framework with GSA. In an earlier work, we demonstrated how the parameters describing the (subjective) distributions can be subjected to sensitivity screening as well (Blanco, Cucurachi, Guinée et al., 2020). This approach has also been described by Lo Piano et al. (2022) and Puy et al. (2020).

4.4 | Other forms of uncertainty

Stirling and other authors have contributed to an important body of work expanding our interpretation of uncertainty and how it manifests in different forms and across different domains (Funtowicz & Ravetz, 1990; Scoones & Stirling, 2020; Stirling, 2010; Wynne, 1992). In this work, we demonstrated the use of forms of uncertainty that are familiar to SSbD modelers (one in which knowledge about the likelihood of relevant events is not problematic). However, it has been argued that "deeper" forms of uncertainty and hidden biases, as well as areas of absolute ignorance, lie outside the models and framings of the problems they are purported to solve. The need for a broader approach to uncertainty emerges in a so-called "post-normal science" (PNS) age, a concept first developed by Funtowicz and Ravetz (1990) to describe a situation in which "facts are uncertain, values in dispute, stakes high and decisions urgent."

When confronted with a PNS context, we first note that the main goal of our proposed framework is to guide R&D toward safer and more sustainable market-ready versions of the technologies before they are deployed at large-scale. Our framework's applicability resides exclusively within the R&D process, which serves as a testing ground. Therefore, the stakes are not as high as when large-scale deployment is imminent and the technology's SSbD qualities are poorly understood. This is the main motivation for early-stage SSbD assessments. Nevertheless, our framework goes beyond conventional SSbD modeling approaches by taking significant steps toward PNS-readiness. Global sensitivity analysis and sensitivity auditing have been demonstrated as powerful tools to unmask hidden biases (Razavi et al., 2021). Furthermore, Bayesian approaches bring the subjective elements of uncertainty analysis to the front, making them explicit and available for rigorous scrutiny by stakeholders. At the same time, they mathematically balance prior subjective beliefs with new incoming data. Conservative uncertainty quantification and Bayesian analysis can help bridge the gap between Stirling's "uncertainty" and "risk" factor types. As a final point here, we note that the framework can also be coupled with complex system models (Borgonovo et al., 2022).

4.5 | Application within the European Commission's SSbD framework

The EC SSbD framework (Abbate et al., 2024; Caldeira et al., 2022) provides a basis for integrating the approach we present. While it lacks detailed guidance for prospective modeling and handling of related uncertainties, it recognizes the necessity of these elements and points to pertinent literature (see Box 1 in Caldeira et al., 2022). Our proposed approach aligns well with the current form of the EC framework, namely Step 3: "Human Health and Environmental Aspects in the Final Application Phase" and Step 4 "Environmental Sustainability Assessment," which require more comprehensive assessments.

Our proposed framework differs from the EC framework in two important ways. First, it focuses on the technology rather than the chemicals or materials that comprise it. The EC framework focuses on the life cycles of chemicals and materials and then indicates that relevant applications of these chemicals and materials (use phase in LCA) should be considered. How this is done, for example, which applications, by whom, and how they are evaluated v*is-à-vis* is an aspect that has not been clearly resolved by the EC framework in our view, and evaluating the life cycle of a material in isolation from its ultimate function can be problematic (Guinée et al., 2022).

Second, our approach is intended to be an ongoing evaluation throughout the R&D journey, from low TRL to TRL 9, rather than snapshot assessments conducted at discrete moments in time (tiers and gates). By continuously updating prospective models as R&D progresses and uncertainty decreases, our approach better fits the dynamic R&D process. A constantly evolving model can be queried and updated at pertinent times by innovators. This also suggests that if something such as SSbD certification were to be conceived, it would perhaps more easily be applied to the R&D *practices* of the innovation company rather than to the final *product*. SSbD practices would optimize the path to TRL9 for safety and sustainability, preparing the product to meet the required standards before market entry. We believe our work, which focuses on the technology's application and the uncertainties driving its innovation process, can stimulate a productive debate on optimizing and strengthening the EC SSbD framework as it continues to develop.

5 | CONCLUSIONS

We conclude with what should be the beginning, which is the nature of the research question faced by SSbD modelers. One can imagine that policymakers and technology developers would ask them: "Given the best information available, what do you think are the most effective strategies to design, produce, use and dispose of this technology in a safe and sustainable way?" Thus, we return to Section 2.3: This is essentially a Bayesian question. The framing we proposed here enables us to translate our best estimates to probability distributions and to systematically and robustly identify the choices that can be made at the R&D stage and that may more profoundly influence the technology in a desired way.

We also recall the popular expression "you are only as strong as your weakest link," which has great relevance in the context of prospective assessments for SSbD. If an element of the LCA or risk model is much more sensitive than the rest, then there is a high chance that the benefits of increased accuracy and precision in the other factors of the model are lost. If great effort is spent in modifying a factor that has only limited influence on the environmental outcomes, then this effort may well be lost. Scenario analysis has proven to be a useful tool in prospective assessments; however, with the proposed framework, we are pushing back against overreliance on scenario analysis without a previous and comprehensive sensitivity screening. Selecting scenarios based only on preconceived notions may often result in that the compared scenarios are not significantly different and therefore are not useful to act upon. This would futilely shift an already stretched focus from decision-makers toward aspects that are ultimately unimportant.

Our framework successfully addresses this shortcoming with robust comprehensive and quantitative methods to support SSbD decision-making. It also offers a useful ontology for the exchange of information between SSbD modelers and technology developers throughout the R&D process. Furthermore, it iteratively simplifies models by allowing non-influential factors to be fixed. Less complex models will allow for clearer and more meaningful analysis, as well as more transparent communication, discussion of the findings, and effective decision-making by all stakeholders.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon request.

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