Chapter 6

A framework for guiding Safe and Sustainable-by-Design innovations

Abstract

Assessing the safety and sustainability of technologies while they are still in early research & 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 developers attempt to optimise material choices and configurations. As designs evolve quickly, assessing their environmental impacts while numerous factors remain undetermined is not straightforward. Thus, assessors often revert to evaluating a limited subset of possible scenarios which are then used to guide design choices. However, selecting scenarios for hundreds of undetermined factors without a systematic sensitivity screening may preclude important improvement opportunities. To provide the best guidance, the evaluated scenarios should be defined by the factors that are most influential on the future environmental impacts of the technology. In this chapter we propose a broad approach that accomplishes this by incorporating a wide spectrum of undetermined factors –both intrinsic and extrinsic to the technology design– in integrated assessment models. These models are then screened for highly sensitive factors using global sensitivity analysis. Strategies to further reduce uncertainty on the most influential factors are proposed for a second iteration, and the residual factors for which uncertainty cannot be further reduced and remain influential are selected as a basis for development of "sensitive" scenarios. We demonstrate the framework by applying it to the life cycle assessment and ecological risk assessment of an emerging photovoltaic technology.

Keywords: life cycle assessment, ecological risk assessment, emerging PV, safe-by-design, sustainable-by-design

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6.1. Introduction

Safety and sustainability criteria are taking an increasingly central role in guiding policy decisions for supporting and regulating new technology development.[1] To better support decision-making during the early research and development (R&D) stages, safety and sustainability practitioners have scrambled to propose diverse prospective methods and criteria such as *ex-ante* LCA[2] and prospective risk assessment.[3] However, there is an important challenge in producing such environmental indicators, i.e. accounting for the uncertain evolution of technical, environmental and socioeconomic factors – both intrinsic and extrinsic to the technologies – that influence the future environmental implications of the technologies once they are deployed at commercial scale[2–6].

Traditional *ex-post* assessments of well-established technologies are already prone to inaccuracy and/or imprecision due to uncertainty and variability.[7,8] A risk/impact estimate may deviate from its actual value in response to spatial and temporal variability of the underlying processes, as well as imprecise or unavailable data regarding the technology's design and operational parameters.[9–11] Errors may also be introduced in the broader environmental impact/risk assessment models, which are composed of mathematical relationships that can only offer limited approximations.[12] 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 *ex-ante*/prospective assessments.[13]

To further illustrate this challenge, we take the case of an emerging photovoltaic technology, III-V/Si tandem cells (III-V/Si).[14,15] These cells have achieved record conversion efficiencies by adding layers of elements from groups III and V of the periodic table (e.g. gallium, indium, arsenic) on top of a silicon substrate to increase light absorption. However, especially the use of arsenic may raise concerns about the safety and sustainability of III-V/Si. Whether the trade-off between potential toxicity and improved solar cell performance is desirable depends on many factors. For example, at end-of-life (EOL) the panels could be recycled, and the arsenic recovered, or they could be incinerated or disposed of in a landfill or underground waste deposit. The extent to which arsenic is recovered from PV panels at EOL will depend on economic factors along with regulatory concerns surrounding e-waste or supply risks.[16,17] Finally, there will be the ease and feasibility of current and future methods for physically separating the arsenic from the other panel constituents will be determinant. Since arsenic can take various forms once released, from high-toxicity (+3 oxidation) to a low-toxicity (methylated) state, uncertainty regarding the form of arsenic to which organisms are ultimately exposed will also be of importance.

The influence of these numerous and interrelated factors which span multiple domains will remain unknown until the assessments are conducted and complemented with some form of sensitivity analysis[18]. A common strategy that has been applied across numerous modelling disciplines to deal with uncertain factors of presupposed relevance is scenario analysis. This approach has provided more confidence in the assessments, 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 even hundreds, especially when considering interactions across social, technical, and economic domains that influence a technology's performance. What is often observed in practice is that a handful of scenarios are selected, which can help as a benchmarking exercise and to identify hotspots.[19,20] In this approach, however, the actual relevance of the selected scenarios to safety and sustainability implications is not evaluated before they are selected, whilst leaving potentially important scenarios outside of the analysis.

In this chapter, we present a framework 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 towards safe and sustainable-by-design (SSbD) innovation. We illustrate the framework by diving deeper into the case study of III-V/Si cells introduced above. The framework follows five steps (Figure 6-1): i) identify and map uncertain factors, with special attention to those specific to the forward-looking or *ex-ante* nature of the assessments; (ii) propose methods for the characterization and propagation of the uncertainties in these factors; (iii) identify the least sensitive factors and fix them to reduce model complexity (iv) apply strategies to reduce uncertainty in the most sensitive factors; (v) in a second iteration, select remaining sensitive factors as a basis to develop relevant scenarios based on sensitivity, e.g. “sensitive scenarios”. Sensitive scenarios will highlight opportunities for most effective safety and sustainability improvements for technology designs that are in the early R&D.

We developed this framework considering two different types of environmental assessments: life cycle assessment (LCA), and human and ecological risk assessment

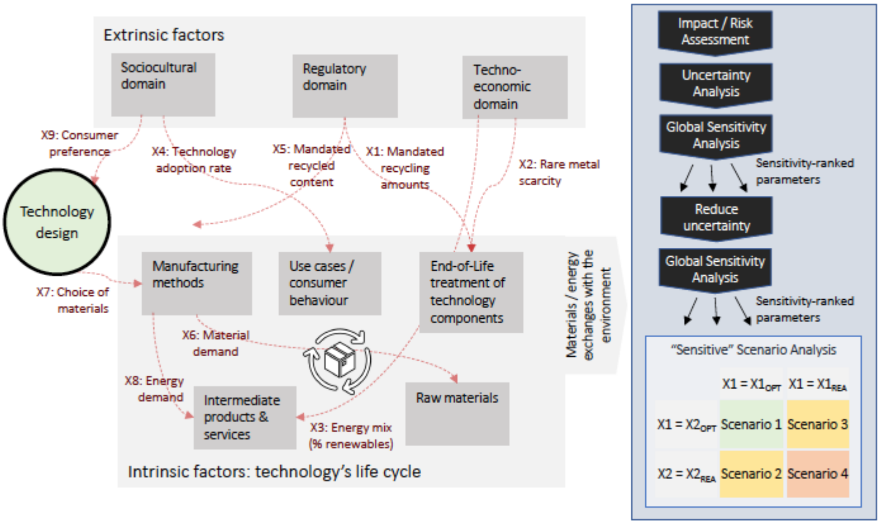

Figure 6-1 Framework for guiding safe and sustainable-by-design innovation. Red arrows show examples of uncertain/evolving factors (X#) that may influence the material and energy exchanges associated to the technology's life cycle, and the concomitant impacts and risks. Global Sensitivity Analysis (GSA) can be used to prioritize the most influential factors for targeting at the design stage.

(HERA). An introduction to each is provided by Guinée et al.[21] and ECHA[22], respectively. The combined use of LCA and HERA is seen as a promising approach for addressing the potential environmental concerns of emerging technologies[23,24]. Although we focus on these two methods, the framework we propose can be applied to other types of technology assessment models.

6.2. Methodological framework

6.2.1. Factors that determine the future environmental performance of emerging technologies

The adoption of a new technology by society will trigger changes in the environment. These changes – whether desirable or undesirable – are quantified using indicators such as concentration of pollutants in air, area of ecosystem degraded, or risk quotients for endpoints such as aquatic species reproduction. Indicators vary in response to changes in factors that interact across different domains, forming a cause-effect chain (Figure 6-1, left). Some factors are farther removed from the technology design itself but may have a larger influence on the indicator. For example, they can reside in regulatory trends, which may set increasingly strict limitations on materials usage, or in social/economic/cultural trends, which may determine how much of the technology is used and where. In an LCA model, for example, a factor such as X8 may represent the amount of electricity that will be required by a chosen manufacturing method (X7). A change either in X8 or X7 will mediate the quantity of CO_2 emitted, but this also depends on the source of electricity that is supplied (X3). These relationships -amongst others- determine the technology's carbon footprint. Extrapolating this analysis to entire life cycles and related processes in the socioeconomic domains, as well as to other types of indicators beyond carbon footprint, makes evident that the number of cause-effect chains and the undetermined factors within them may easily fall in the hundreds or thousands.

6.2.2. Sources of uncertainty in models of the future

Uncertainty has been comprehensively studied in *ex-post* assessment models. A good overview is provided by Lloyd and Ries[25], who classify uncertainties according to different LCA modelling components: parameter (input data), model (mathematical relationships), and scenario (normative choices). A similar set of uncertainty sources has been described in risk assessment[26]. *Ex-ante* assessments introduce additional sources of uncertainty due to the forward-looking nature of the assessments. Table 6-1 extends our previous work[13] and proposes a comprehensive typology for these new sources, along with relevant examples found in both HERA and LCA *ex-ante* models. It is important to note that there can be overlap between uncertainty types. 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 even 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.

6.2.3. Model parametrization: putting uncertainty types at the same level

The first step in our framework is to translate as many uncertainties as possible to a parameter type of uncertainty. This requires all potentially influential factors, such as those listed in Table 6-1 to be represented as variable parameters in a single integrated model. This is straightforward for the "parameter" types of uncertainties listed. Scenario uncertainties of type I, III, V and VII, which are often assessed independently, can also be parametrized using the approach we demonstrated in Chapter 4, where alternative scenarios exist simultaneously in a model and are activated or deactivated stochastically using binomially distributed parameters as triggers.[13] Model uncertainties can be incorporated in a similar way, as described by Saltelli et al.[27] and Mendoza-Beltrán et al.[28]

6.2.4. Characterization of *ex-ante* uncertainty

The second step involves expressing the range of possible values for all parameters - including triggers for alternative models and scenarios- as probability distributions. Since we are referring to future events, we must first specify what is meant by probability. We will advocate for a Bayesian interpretation of probability, but briefly describe other approaches as well to support our case:

- A *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 so the approach is of limited use in *ex-ante* assessments.
- The *classical* approach determines the likelihood of occurrence of each value, based on all possible values. This approach can be useful in *ex-ante* assessments, e.g., if we know beforehand that there are only three possible processing routes for a given component of the technology. This gives each route 1/3 chance of success. An important limitation of this approach is that all possible values are given equal odds of occurrence.
- The *Bayesian* or *subjective* approach uses probability distributions to represent the degree of belief that an observer has in a particular outcome.[29,30] The Bayesian approach has been applied in risk assessment[31] and to a lesser extent in LCA[32]. It is especially useful for *ex-ante* assessment, if not essential; many possible future states cannot be simulated in a frequentist way. While frequentists have long argued that subjectivity is a strong limitation (or outright invalidating the scientific nature of the exercise), it is also a key strength in that it incorporates other sources of relevant information where actual measurement data is scant or unavailable. Bayes' Theorem provides a formal method for updating the beliefs (represented by so-called *prior* probability distributions) once new data becomes available to produce a *posterior* distribution.[30] This naturally fits the research & development process, which iterates a technology through additional testing and gradual upscaling in order to optimize it until it is ready for commercialization.

The question then is how best to establish prior distributions for uncertainties and variabilities of the types listed in Table 6-1, and then how to update them. Prior distributions must reflect beliefs about parameters that describe the uncertainty of the true (future) state of a factor, e.g., the probability that manufacturing method A will be used instead of B for a particular component once the technology reaches industrial scale. The most conservative attempt would be to start with flat or "non-informative" prior distributions, which distribute probabilities evenly across all possible parameter values. However, there is a trade-off regarding how informative subsequent posteriors will be. Wolpert et al.[33] describe this situation very well 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.[33]

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, i.e. a PERT prior probability density function will be updated to a PERT posterior probability density function.[30] Conjugate priors also make the estimation of posterior distributions a far simpler and more intuitive exercise once additional data or observations are obtained (see Box 6-1).

6.2.5. Propagation of uncertainty and variability

Two approaches for propagating uncertainties are commonly applied; analytic and numerical[34]. 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.[35] The preferable alternative is Monte Carlo simulation[36,37], which generates 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. The frequency distribution of the obtained values is used to construct a probability distribution.

When propagating uncertainty, it is often the case that two or more elements in a model share a source of uncertainty. When this happens, the values for both parameters are dependent.[35] Correlations have been identified between many elements of *ex-post* LCA models.[38,39] They also exist amongst the *ex-ante* uncertain parameters listed in Table 6-1. For example, a future increase in ambient temperature may affect the amount of cooling needed to safely operate a novel battery technology, increasing energy consumption and CO_2 emissions of the system. The same factor may affect precipitation and cloud cover. Both mechanisms will have a global warming impact that to some extent depends on the same uncertain factor.

Table 6-1 Uncertain factors in ex-ante assessments of emerging technologies. Factors are classified according to their modelling domain and whether they are extrinsic or intrinsic to decision-making during the R&D process.

Type	Domain	Intrins.(I)/ Extrins.(E)	Uncertain factor	Uncertainty type	LCA component	HERA component	Context and examples
I	Technology design	I	Material choice	Scenario	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.[13] (metallization of PV cells)
II	Technology design	I	Material quantity	Parameter	Inventory (foreground)	Emission scenario	Quantities of materials used in the design may vary as the design gets optimized.
III	Technology manufacturing	I	Manufacturing route	Scenario	Inventory (foreground)	Emission scenario	Manufacturing/synthesis methods may change when upscaling to industrial scale. See Picchino et al.[40] (chemicals)
IV	Technology manufacturing	I	Material and energy use	Parameter	Inventory (background)	Emission scenario	Process optimizations likely lead to reduced material and energy consumption. See Cucurachi et al.[41] (silicon PV cells)
V	Techno-economic	E	External industries processes	Scenario	Inventory (background)	Emission scenario	Analogous to (III) but applied to external suppliers.
VI	Techno-economic	E	External industries materials & energy use	Parameter	Inventory (background)	Emission scenario	Analogous to (IV) but applied to external suppliers. See Harpprecht et al.[42] (metals)
VII	Techno-economic	E	External markets composition	Scenario	Inventory (background)	Emission scenario	Changes in market compositions for products and services in the supply chain. See Mendoza-Beltran et al.[43] (energy) and Harpprecht et al.[42] (metals)
VIII	Technology use	I/E	Function of technology	Scenario	Goal and scope	Emission scenario	The technology may ultimately be used in different ways. It may be used for multiple/different purposes. See Hiremath et al.[44] (batteries) and Hischier et al.[45] (engineered nanomaterials).
IX	Technology use	I/E	Survival/Failure rates	Parameter	Inventory (foreground)	Emission scenario	Failures (due to e.g. obsolescence, degradation or misuse) may cut the technological products' lifetimes short. See Miller et al.[46] (online commerce)

Type	Domain	Intrins.(I)/ Extrins.(E)	Uncertain factor	Uncertainty type	LCA component	HERA component	Context and examples
X	Technology use	I	Functional performance	Parameter	Goal and scope	Emission scenario	Operational performance parameters may deviate from expected values. See Gong et al.[47] (perovskite PV).
XI	Technology EOL	I/E	Recycling	Scenario	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[48] (battery recycling)
XII	Regulatory	E	Material use & emission thresholds	Parameter/ scenario	Inventory (background)	Emission scenario	Regulation may impose new limits on emissions, use or choice of materials and energy sources.
XIII	Environment /landscape	E	Characterization model: fate	Parameter	Impact assessment	Fate	Landscape parameters that may affect transport and fate of the substances can change in time, e.g. changing averages for ambient temperatures, wind speeds or ocean water pH can affect how substances are distributed in the environment.
XIV	Environment /landscape	E	Characterization model: exposure	Parameter	Impact assessment	Exposure	Parameters that affect exposure e.g. population densities or diets can change in time.
XV	Environment /landscape	E	Characterization model: effect	Model	Impact assessment	Effect	Marginal changes may result in exponentially larger effects as the baseline condition deteriorates. e.g. impact of increased radiative forcing on ecosystems.
XVI	Techno-economic	E	Allocation	Parameter	Inventory (foreground)	N.A.	The parameters used to establish the criteria for allocation of multifunctional processes may change in time. e.g. forecasted market values in the case of economic allocation in LCA.
XVII	Techno-economic	E	Resources	Parameter	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.[49] (water scarcity)

Integrating models presents an important opportunity to account for dependencies between parameters across different processes, scales and domains. This is not trivial to our goal: a factor that has dependencies can have additional indirect influence on the model's output, i.e., it may become more relevant. A convenient way to address correlations is to isolate each shared source of uncertainty or variability in one single parameter. The random values for the Monte Carlo simulation can be pre-sampled, ensuring the same value for all occurring instances of the shared parameter is used within each Monte Carlo run.[50] This strategy already prepares the data required for the next step.

6.2.6. Global sensitivity analysis: screening for relevant factors

A global sensitivity analysis (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"[51]. 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 uncertainty parameters. This requires calculation algorithms for sensitivity indices 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 in Chapter 5), which makes analytical GSA methods not practicable. "Black box" or model-independent GSA methods such as the *delta* measure introduced by Borgonovo[52] are thus favoured. Third, the introduction of binomial and other discrete distributions for parameters may sometimes result in multimodal output distributions. Therefore, variance-based methods may not be suitable and moment-independent methods are preferred.[52,53]

As we showed in Chapter 4, and elsewhere[13,41], one GSA method that meets these requirements is the Borgonovo delta sensitivity measure[54]. The Borgonovo *delta* represents the influence of a parameter as its ability to shift the model's output distribution curve. This is illustrated by Figure 6-2, where the red 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 (*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 value assumed by the parameter) and will become narrower (lower uncertainty/dispersion in the model output or risk score). The new blue curve (conditional) is the environmental risk for the specified scenario. For an environmental indicator, it is usually desirable that the output distribution curve moves towards the origin on the x-axis (lower risk/impact) and becomes narrower (less uncertainty). The curve *shift* is defined by Borgonovo as the non-overlapping area between both curves. The *delta* sensitivity measure is the probability-weighted average of all possible shifts induced by the parameter when it is fixed at its possible values.[54]

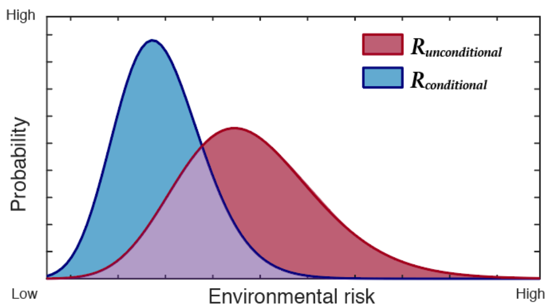

Figure 6-2 Graphical representation of Borgonovo's delta sensitivity measure in an environmental model. The non-overlapping area (blue + red) represents the shift in the curve when the model is evaluated conditional to an uncertain fixed at one of its possible values (Adapted from Borgonovo[52]).

6.2.7. Second iteration: further reducing uncertainty

The first GSA iteration may result in several factors that have higher sensitivity. Before producing recommendations or making any decisions on the technology design, three avenues can be used first to further reduce uncertainty in the model. For subjective probabilities: structured expert knowledge elicitation protocols such as DELHPI, aimed at reducing bias while furthering consensus[55,56]. Some of these methods have even been extended to incorporate the experts' beliefs regarding their own uncertainty[57–59] For other uncertain factors, more refined modelling can be applied specifically to the nature of the parameter, e.g. hydrological, geochemical, or economic models based on market research. A third recourse is to collect additional data from lab or pilot-scale tests, such as leaching tests or process consumption and emissions measurements. Bayesian inference can then be used to update the probability distributions for the factors for which new data was obtained (see Box 6-1).

6.2.8. Proposing safe and sustainable by design strategies

Once the possibilities to further reduce uncertainty have been exhausted, a second uncertainty propagation and GSA iteration will produce the residual most relevant factors. These factors can then be used to construct "sensitive" scenarios, which by this point will likely consist of a much smaller, but highly relevant subset. These 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 changes and/or other measures that can be taken to show the most efficient measures towards a safe and sustainable deployment of the technology.

The sensitive scenarios point to the factors which are most influential *while still subject to considerable change*. This presents an opportunity to influence these factors by attempting to fix them at a desirable value or at least reduce their uncertainty/variability towards a smaller and more desirable range (shift the distribution to the left and make it narrower). Because the factors can span different model domains, their nature may vary significantly as will the possible ways to influence them. A well-tested guiding principle that has been applied for several decades in risk management is the hierarchy of risk control measures, which leads the decision-maker to prioritize strategies according to the order (i) elimination, (ii) substitution, (iii) engineering control, (iv) procedural control and (v) personal protective equipment. Such strategies are already very visible in proposals for emerging PV technologies, such as in-situ sequestration of lead in perovskite solar cells[60] (engineering control), replacement of lead for tin (substitution)[61], and administrative management of the risk (e-waste regulations[17,62]).

6.3.Case study of an emerging solar energy technology

6.3.1. III-V/Si photovoltaic system

To demonstrate the proposed framework, we apply it to the III-V/Si PV technology. In Chapter 3 we conducted a life cycle assessment of this technology largely based on lab-scale and pilot data from a European R&D project.[63,64] In the following sections we take this as a starting point and develop the different steps of the framework. The iterations result in different versions of the LCA and RA models, each representing our state of knowledge at different points in time as the R&D project advanced.

6.3.2. Life cycle assessment

The manufacturing of III-V/Si cells involves numerous processing steps, most of which are already at industrial scale and used in the mainstream silicon PV industry. Two key steps, however, are still early-stage concepts which could only be tested at lab and pilot-scale. The first is the deposition of the top cell's III-V layers, which are grown via Metalorganic Vapour Phase Epitaxy (MOVPE).[65] In the initial phase of the project (*t=0*) we considered state-of-the-art MOVPE reactors that are currently used in related industries. These reactors have a high energy consumption with low throughputs (7 round 4" wafers per run at 3.5-hour runtime). For a future III-V/Si PV industry, this would not be economically viable or environmentally advantageous.[64] Therefore, this was an R&D priority and by the end of the project (*t=1*), a pilot-scale reactor achieved a throughput of 31 round 4" wafers per run at 2.5 hours runtime.

It was determined, however, that even larger throughputs would be required to make the technology economically feasible. Further projections of throughput increase and runtime reductions were elicited from experts, based on what they would consider feasible future improvements in the reactor (*t=2*). Such improvements include switching to larger wafers (square M2 wafers) and increasing throughput to 50 wafers per run at 0.5 hours runtime. A PERT distribution was used to represent this uncertain evolution via two factors: MOVPE power consumption per wafer area and MOVPE process runtime. The distributions' minimum, mode and maximum parameters were adjusted accordingly between *t=0* and *t=2* based on the R&D achievements and experts' projections for what would ultimately be feasible.

The second key processing step is the metallization of the front contacts, for which a decision had to be made between nanosilver and nanocopper ink as described in Chapter 4.[13] The analysis made in this previous work represented the state of knowledge at an initial state of the project (*t=0*). Additional research and testing were conducted, showing more promising results for copper. We use this Boolean factor to illustrate Bayesian updating within the framework (see Box 6-1) and how it can be updated in an intermediate step (*t=1*) and towards the end of the project (*t=2*) based on the results of lab tests.

Box 6-1 – Bayesian updating applied to uncertainty in material compositions

In building an *ex-ante* LCA of an emerging photovoltaic cell design, it was found that two alternative materials for the front metallic contacts were under consideration: nanosilver and nanocopper particles.[13] The material that shows best electrical properties will ultimately be incorporated in the cell design, but this may depend on evolving intrinsic and extrinsic factors. Thus, we want to use a probability distribution to represent the chance of copper performing better than silver, so that the choice of material can be used in a probabilistic LCA model. The competition between copper and silver can be simulated as a binomial process, where the success of copper over silver in any given trial is described by Equation 6-1:

$x \sim bin(1, p)$ (Eq. 6-1)

If copper is successful, $\boldsymbol{x}$ will take a value of 1 while if silver is successful, $\boldsymbol{x}$ will take a value of 0. The uncertain parameter of interest is $\boldsymbol{p}$, which is the probability of copper having better properties than silver in a random trial*. We don't know this probability and must make a subjective estimate of it. The data we have is the following: Six trials have been conducted to date. Copper showed better properties (success) on 4 of the 6 trials.

Establishing a prior: Choosing a beta distribution to describe $\boldsymbol{p}$ greatly simplifies inference of binomial parameters.* From the data we have, we set the mean $\boldsymbol{\mu}$=4/6 from a sample size $\boldsymbol{n}$=6. The parameters $\boldsymbol{\alpha_0}$ and $\boldsymbol{\beta_0}$ of the (prior) beta distribution for $\boldsymbol{p}$ can be calculated from $\boldsymbol{\mu}$ and $\boldsymbol{n}$ using Equations 6-2 and 6-3. Our prior beta distribution for $\boldsymbol{p}$ is then specified by parameters $\boldsymbol{\alpha_0}$ = 4 and $\boldsymbol{\beta_0}$ = 2 (Figure 6-3, "Prior").

$\alpha_0 = \mu \cdot n$ (Eq. 6-2) $\beta_0 = (1 - \mu) \cdot n$ (Eq. 6-3)

Updating to a posterior: A posterior distribution for $\boldsymbol{p}$ can be obtained when additional testing is performed. Following the analytical updating procedure of DeGroot[66], if 3 additional laboratory tests (trials) are performed and copper shows better performance in 2 out of 3 tests, the posterior distribution (Figure 6-3, Post1) will also have a beta form, this time with $\boldsymbol{\alpha_1} = \alpha_0 + 2$ and $\boldsymbol{\beta_1} = \beta_0 + 1$. Here, 2 and 1 represent successes and failures of copper to perform better than silver in the new trials, respectively. If an additional test is performed where copper is again successful, we again update our posterior beta distribution (Post2) with $\alpha_2 = \alpha_1 + 1$ and $\beta_2 = \beta_1 + 0$ (Post2).

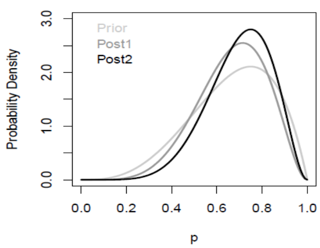

Figure 6-3 Bayesian updating of the probability of success of copper over silver

The x-axis in Figure 6-3 plots $\boldsymbol{p}$, which is the chance of success of copper, and the y-axis plots the probability of the x-value for parameter $\boldsymbol{p}$ being correct. Updating $\boldsymbol{p}$ with new test results moves the chances in favour of copper but also reduces the spread of the distribution curve.

Some additional parameters in the background silicon supply chain and other non-cell components were also updated between *t=0* and *t=2* to better reflect state-or-the-art, following the work of Cucurachi et al.[41] Table 6-2 summarizes how we represented the evolution of these factors in the model using different probability distributions.

The resulting impact score distributions for climate change for each snapshot of the technology is shown in Figure 6-4. The figure clearly illustrates how successive iterations reduce not only the impact (by any measure of central tendency) but the dispersion as well. The Bayesian updating of the front metallization route in favour of copper with a laser sintering route shifted the distribution slightly to the left and reduced dispersion at *t=1*. In the final period of the R&D project (*t=2*), two key achievements resulted in a significant improvement and reduction in uncertainty: the successful demonstration of the pilot reactor with significantly lower power requirements, and the decision to fully abandon the silver metallization route as well as the chemical sintering method in favour of the copper with laser sintering route.

In the first iteration (*t=0*), the global sensitivity analysis (Figure 6-5) 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). A second tier of importance consisted of several factors 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 (*p1-p5*). In the case of binomially distributed factors, the underlying probabilities p_x of each were more influential than the factors themselves. This contrasts with the result we had obtained for similar distributions in the simplified case study of Chapter 4.

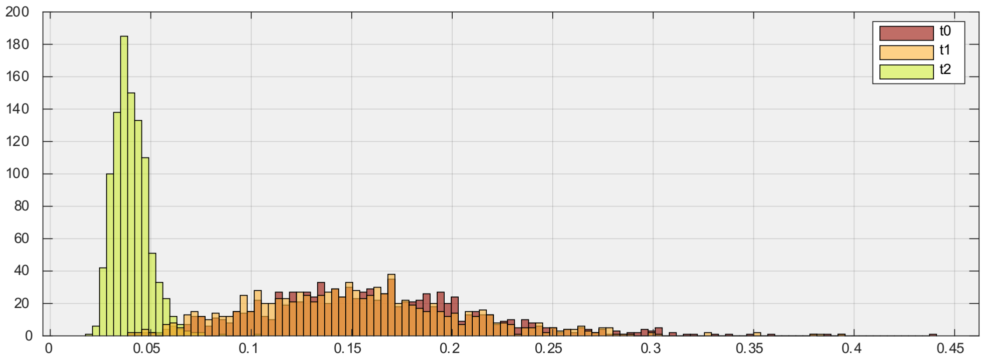

Figure 6-4 Frequency distribution for climate change impact scores (in kg CO2 eq) of the emerging III-V/Si technology in three successive snapshots in time: t0=midpoint through the R&D project, t1=after additional lab tests for different front metallization configurations, and t2=at the end of the R&D project.

[*] See Table 6-2 for factor/parameter definitions.

Table 6-2 - Evolution of key factors in an LCA model of the III-V/Si tandem photovoltaic technology

Factor Id	Factor description	Initial model (t=0)	Final model (t=2)
MOVPE			
P_movpe	MOVPE tool power load per processed wafer area	pert (min=1, mode=509, max=509, shape=4)	pert(min=13.3, mode=119, max=119, shape=4)
RT_movpe	MOVPE runtime	pert(min=0.5, mode=3.5, max=3.5)	pert(min=0.5, mode=1, max=2.5)
Scru_cons	Scrubber granulate consumption	triang(min=2.55, mode=7.65, max=7.65)	No change
Front metal*			
Cu_v_Ag	Choice of Cu nanoink vs. Ag nanoink	bin(1, p_1) p_1 ~ beta(4,2)	1 (resolved)
Synth_Ag	Choice of chemical vs physical synthesis for Ag	bin(1, p_2) p_2 ~ pert(1000, 0.5,0.7,0.8)	N/A
Synth_Cu	Choice of chemical vs physical synthesis for Cu	bin(1, p_3) p_3 ~ pert(1000, 0.5,0.7,0.8)	No change
Sint_Cu	Choice of laser vs. chemical sintering for Cu	bin(1, p_4); p_4 ~ pert(min=0.1, mode=0.2, max=0.3, shape=4)	1 (resolved)
Sint_Ag	Choice of laser vs. chemical sintering for Ag	bin(1, p_5); p_5 ~ unif(1000, 0,1)	N/A
Performance parameters			
Eff_panel	Panel efficiency	pert(min=0.25, mode=0.28, max=0.31, shape=4)	No change
PR_syst	Performance ratio of PV system	pert(min=0.8, mode=0.85, max=0.9, shape=4)	No change
LT_panel	Panel lifetime	norm(30, 5)	No change
Background supply chain			
Cu_scrub	Scrubber granulate copper fraction	pert(min=0.2, mode=0.3, max=0.7, shape=4)	No change
Cu_rec	Recycling of copper from granulate	bin(n=1, p= 0.5)	No change
Al_panel	Aluminium in panel	lnorm(gm= 2.63, gsd=1)	unif(1000, min=1.6, max=2)
Glass_panel	Glass in panel	lnorm(gm=10.08, gsd=1.22)	unif(1000, min=5.04, max=7.56)
Elec_panel	Electricity to manufacture panel	lnorm(gm=4.71, gsd=1)	unif(1000, min=12.22, max=15.27)
Elec_siem	Electricity consumption Siemens process	lnorm(gm=110, gsd=1)	unif(1000, min=34.1, max=44.3)
Heat_siem	Heat consumption Siemens process	lnorm(gm=185, gsd=1)	unif(1000, min=57.24, max=74.52)
Elec_CZ	Electricity consumption Czochralski process	lnorm(gm=85.6, gsd=1.22)	unif(1000, min=43.4, max=69.3)
Si_CZ	Silicon consumption for Czochralski process	lnorm(gm=1.07, gsd=1)	triang(1000, min=0.4, mode=0.66, max=0.75)

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.

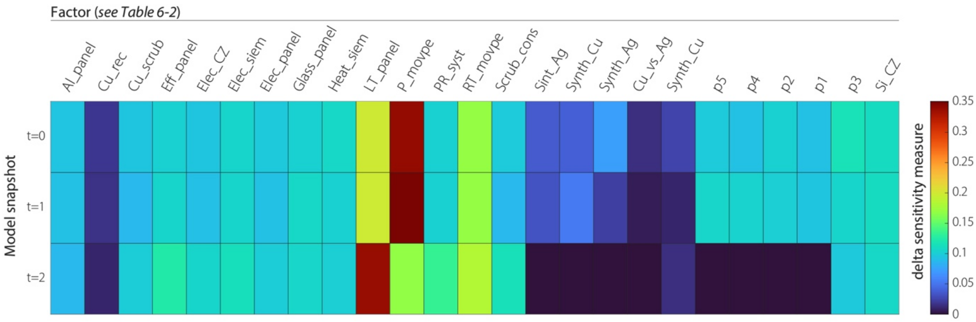

Figure 6-5 Delta sensitivity measures (relative to other factors) in three successive snapshots in time: t=0: midpoint through the R&D project, t=1: after additional lab tests for different front metal configurations, and t=2: at the end of the R&D project. The description of each factor is provided in Table 6-2.

At the end of the R&D project (*t=2)*, the influence of MOVPE power consumption is largely reduced and the most sensitive factor by a considerable margin is now the panel's lifetime. This presents an interesting opportunity; on one hand, III-V cells have been designed in the past to withstand extreme radiation for their applications in space and there is a good case for III-V/Si cells to last longer than conventional silicon ones. Following the hierarchy of risk controls suggested in section 6.2.8, 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 end-of-life.

6.3.3. Risk assessment

In Chapter 5 we conducted a detailed prospective ecological risk assessment of the III-V/silicon tandem PV technology throughout its various life cycle stages, with a focus on the III-V materials that constitute the top cell (gallium, arsenide, indium). The model underpinning the assessment presented reflects the current state-of-knowledge and concluded that the risks are low to negligible in the explored scenarios. An earlier preliminary version of the assessment was conducted ca. 2 years earlier with more limited knowledge.[67] Here we present for illustration purposes how this first version of the model was refined and how the conclusions changed considerably after applying the framework. The key model settings and assumptions that changed are described in Table 6-3.

Figure 6-6 shows the distribution for the risk quotient obtained for arsenic emissions to soil in a no-recycling scenario (no arsenic recovered from PV panels collected for disposal). A global sensitivity analysis of this preliminary model 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 final 2 years of the R&D program. The model was refined as presented in Chapter 5, with leaching processes reparametrized in terms of a solid/waste partitioning coefficient (k_{sw}) for which more than 100 datapoints were available. Leakage processes were also reparametrized in terms of landfill infiltration, for which again more than 100 datapoints were available.

Table 6-3 - Evolution of key factors in the ecological risk assessment model of the III-V/Si tandem photovoltaic technology

Factor description	Preliminary model (t=0)	Current model (t=1)	Future model (t=2)
PV capacity demand	Steady state 5 GW capacity addition per year	Dynamic, logistic growth curve based on >1000 datapoints.	No change
Arsenic waste leaching in landfill	Constant rate (% mass/year). Empirical, based on two datapoints, a lognormal distribution was assumed with mean 0.8 and variance 0.3.	Dynamic, calculated from empirical solid/waste partitioning coefficient (k_{sw}) based on >100 datapoints.	Leachate pH controlled resulting in higher k_{sw} (now sampled only from the upper quartile of the distribution used in t=1).
Leakage of landfill leachate to surrounding soil compartment	Constant leakage rate of landfill leachate to the surrounding soil compartment (%/year): based on 1 datum, a lognormal distribution was assumed with mean 2.0 and variance 0.7.	Constant, calculated from landfill infiltration rates based on >100 datapoints.	No change
Landfill cell depth	Not applicable	Empirical, exponential distribution with a peak at 10 and lower value 0.5m. based on >100 datapoints.	Increased landfill depths (PERT distribution with min=5, mode=7.5 max=10 m.)
Recycling rate	85%-99.9% panels collected	85%-99.9% panels collected	Increased to 95%-99.9% panels collected
Incinerator abatement	98-99.9% arsenic captured in electrostatic precipitator	No change	Improved to 99.5-99.9% arsenic captured in electrostatic precipitator

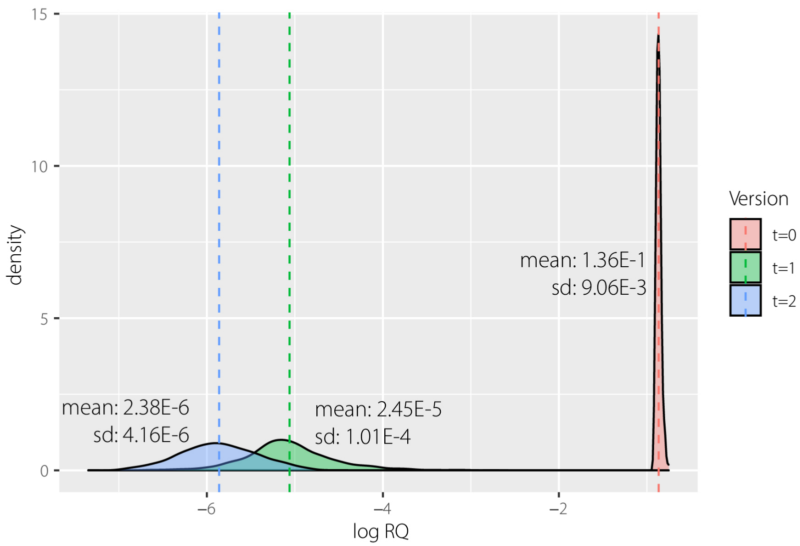

Figure 6-6 Frequency distribution of risk quotient for III-V/Si arsenic emissions to soil in the European continent

Both processes -along with the growth in PV demand- were modelled dynamically rather than steady-state, recognizing the relevance of the temporal dimension and to reflect more realistic scenarios. As a result, the risk quotient for arsenic in the soil compartment in Europe was reduced by several orders of magnitude, becoming negligible. We note that dispersion increased considerably with the model refinement that took place between *t=0* and *t=1*. This is likely attributed to the refined landfill model where the new parameters – especially the waste/leachate partitioning coefficient - introduced a large variability. Arguably, it is best to first improve accuracy, even if it at the expense of precision.[12]

The GSA in Chapter 5 (corresponding to *t=1*) pointed to four factors to target and strategies to address them: the waste/leachate partitioning in the landfill, the landfill depth, the recycling rate, and the incinerator abatement. The combined effect of these actions can be evaluated in an "optimistic" future scenario *t=2*, where the risk could be reduced by an additional order of magnitude as a result of specific strategies. Figure 6-6 shows how the risk is further reduced by nearly an order of magnitude.

6.4. Discussion

6.4.1. Insights obtainable through the framework

Applying our framework to the LCA of the III-V/Si PV system highlighted a very interesting point regarding the lifetime of PV panels, which resulted in the most sensitive factor after three iterations. While it is common in LCAs of PV to standardize the lifetime parameter to a fixed value[68] e.g., 25 or 30 years, 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 avenues for more sustainable design. On the other hand, there is the proper maintenance and protection of the panel during its use phase. Together with the decision to use the panel throughout its entire useful life and not replace it earlier than needed, this opportunity is 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 6-5). In a way, these recommendations follow the progression of the hierarchy of risk controls, where engineering controls (design changes) are exhausted and administrative controls (e.g., consumer behaviour) follow next.

To better illustrate the potential implications of improved panel lifetime management, we can observe the shift in the climate change impact score distributions when panel lifetime is fixed at its min (25 years) and max (35 years) values for a pessimistic and optimistic case, respectively. For the distributions in Figure 6-7, the mode shifts from ca. 0.045 in the pessimistic case to 0.03 kg CO2 eq. in the optimistic case, an impressive potential for impact reduction of 33%. After three iterations, the LCA model was simplified from 25 underspecified factors to 15, without ignoring the remaining 10. Rather they were systematically assessed and then fixed at an average value, since their uncertainty was proven unimportant. Of the remaining 15 factors, it would now be justifiable to prioritize 3 or 4 factors (panel lifetime and MOVPE process parameters).

6.4.2. 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 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.[41] 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 a sustainability practitioner 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 practitioner and the technology developer, as we have often observed in practice).

Furthermore, the most time-consuming refinement is expected to happen during the second iteration, 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, e.g., developing and communicating numerous ad-hoc scenarios or developing more detailed modelling such as process engineering upscaling for all

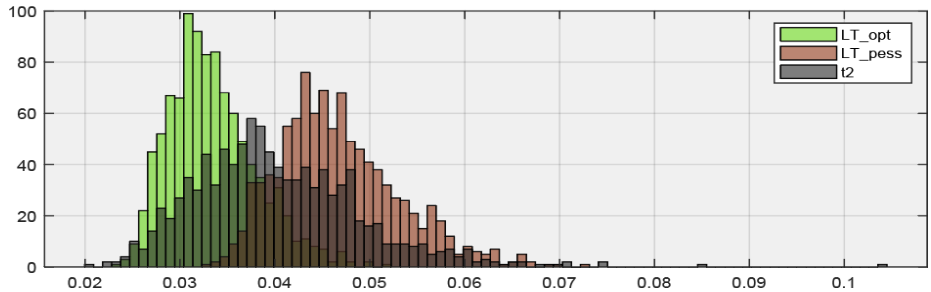

Figure 6-7 Frequency distribution for climate change impact scores (in kg CO2 eq) of the emerging III-V/Si technology in three "sensitive scenarios": with a short panel lifetime of 25 years (LT_pess), with a long panel lifetime of 35 years (LT_opt) and with an uncertain panel lifetime distributed according to the final model at the end of the R&D project.

uncertain parameters. Our framework ensures that the additional resources required by *ex-ante* are devoted to the things that matter.

6.4.3. On subjective probability distributions

Another concern is whether it is realistic, robust, and transparent to introduce largely subjective probability distributions that may cause some confusion about models' operations and outputs. 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. Their effects are systematically introduced, analysed and interpreted. Two types of subjective information are introduced in our framework when subjective distributions are used. First, the shape of the distribution (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 which resembles that of in-line tools used in high-throughput production of commercial silicon cells which have 30 or more years advantage. For a conservative approach, we set the mode equal to the maximum. We could have chosen a triangular shape using this 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 which 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.[13] Interpretation and decision-making will necessarily involve probabilistic weighing, whether it is done by the practitioner 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 *ex-ante* assessments must be conducted in a low-information environment. Therefore, all information available should be used, including beliefs, constraints and plausibilities that narrow the space for ambiguity.

6.5.Conclusions

The popular expression "you are only as strong as your weakest link" has great relevance in the context of *ex-ante* environmental assessments for safe and sustainable designs. If an element of an integrated model has a resolution far coarser than the rest, then there is a high chance that the benefits of increased precision in the rest of the model are lost. In the same way, if great effort is spent in modifying a factor that has only limited influence on the environmental outcomes, then this effort is lost. Scenario analysis has proven to be a useful tool in *ex-ante* assessments; however, with the proposed framework we are pushing back against overreliance on scenario analysis without a previous and comprehensive sensitivity screening. Selecting scenarios to assess only based on preconceived notions may often result in that the compared scenarios are not significantly different therefore are not useful to act upon. This shifts an already stretched focus from decision-makers to aspects that are ultimately unimportant.

Our framework successfully addresses this shortcoming with robust systematic and quantitative methods to support decision-making. It also offers a useful structure for the information exchange between environmental modellers 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 communication and discussion of the findings amongst stakeholders.

There are important improvements of the framework that may be of interest for *ex-ante* LCA and RA researchers to further develop. We particularly see two valuable future developments. First, the incorporation of multivariate Bayesian approaches which can allow inference on more complex or underspecified distributions. Second, the incorporation of strategies to deal with correlations between observations from lab/pilot test results. In combination, these two improvements could significantly strengthen the framework and broaden its applicability.

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