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Guiding safe and sustainable technological innovation under uncertainty: a case study of III-V/silicon photovoltaics

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Chapter 7

General Discussion

7.1. The role of early-stage environmental assessments

Every four years, millions of American voters and keen observers abroad point their web browsers to the *FiveThirtyEight* website, one of the most successful platforms for monitoring and forecasting of presidential U.S. elections.[1] Few events could be more influential to modern society since the second half of the 20th century, and Nate Silver (the site's founder) rose to prominence by applying powerful statistical predictive models to the heated topic with unprecedented success. In perhaps the only enjoyable book ever written about probability and statistics, *The Signal and The Noise: Why Many Predictions Fail – but Some Don't*, Silver -a strong advocate for Bayesian thinking- writes:

> *Good innovators typically think very big and they think very small. New ideas are sometimes found in the most granular details of a problem where few others bother to look. And they are sometimes found when you are doing your most abstract and philosophical thinking, considering why the world is the way that it is and whether there might be an alternative to the dominant paradigm. Rarely can they be found in the temperate latitudes between these two spaces, where we spend 99 percent of our lives. The categorizations and approximations we make in the normal course of our lives are usually good enough to get by, but sometimes we let information that might give us a competitive advantage slip through the cracks. The key is to develop tools and habits so that you are more often looking for ideas and information in the right places-and in honing the skills required to harness them into W's* (wins) *and L's* (losses) *once you've found them.*[2]

If early-stage environmental assessments are to play a contributing role in technological innovation, we must look through the cracks and in the granular details that Silver points to. How can we do this then, in the face of overwhelming dearth of data, rapidly evolving technology designs and limited time to adjust and reinterpret our models? Perhaps the two most challenging aspects of the whole *ex-ante* safety and sustainability assessment exercise are model development and data collection. This gives four approaches to where/how to focus the limited knowledge-gathering resources at our disposal:

a) Rapid screening, based on highly simplified models and limited data collection. This approach has often been the *go-to* for chemical safety of novel materials and various techniques such as *read-across* have been developed.[3]

b) Keep models simple and focus the resources on improving data collection as much as possible. This has often been the approach of practitioners in the rising field of *ex-ante* LCA.[4]

c) Accept uncertainty due to limited data and devote the resources to refine the models as much as possible.

d) Only produce the assessments when the technology is fully developed, allowing for both models and data collection to be refined to the standard of conventional *ex-post* assessments.

Approach (d) runs into the well-documented issues of the *Pacing Problem*[5] and the *Collingridge Dilemma*[6] which were discussed in the introductory chapter of this text. Approach *(a)* entails a high likelihood of producing meaningless results due to a combination both inadequate data and models. Furthermore, while it may be a suitable approach for chemicals which are developed much more rapidly than technological products or services[7], it may fall short in the latter given the difficulty to apply techniques such as *read-across* to entire technological product systems. Approach *(b)* tries to improve on the data but will likely leave us with inadequate explanations if relevant cause-effect mechanisms are omitted. Approach *(c)* on the other hand, opens as many opportunities as possible to improve the technology's design while there is still considerable room for trial and error. The more important role of the early-stage assessment is then that of an *enabler* rather than an arbitrator or judge. Approach *(c)* is very well suited to the task.

7.2. New insights obtained in this work

The five content chapters in this text underpin the perspective presented above and progressively lay the groundwork for an overarching methodological framework that takes important steps in a new direction for early-stage sustainability assessments. The insights obtained in each chapter are summarized below. As anticipated in the introductory chapter, these insights are methodological but also technical in that they contributed to a better understanding of the potential advantages and drawbacks of future large-scale III-V/silicon PV deployment.

- *What are the environmental hotspots in the emerging PV technologies landscape and what are the variabilities in the life cycle impacts?*

Chapter 2 initiates with a high-level investigation of environmental hotspots in the emerging PV landscape. Which PV technologies are presenting comparative hotspots (vs. conventional c-Si PV) and why? A systematic review and meta-analysis of over LCA studies conducted in the past decade found that most hotspots for the emerging PV landscape were found in perovskite cells. While perovskite cells are perhaps the most promising alternative from a cost and energy security perspective, their short lifetime (due to poor stability of the perovskite layer) means increased material intensity and larger environmental drawbacks per kWh of electricity generated. The variabilities in the impacts reported across and within technology types were found to be large, spanning several orders of magnitude despite a considerable effort in harmonizing system boundaries and other aspects of the underlying LCA models. While PV technologies are typically classified according to the light-absorbing materials used in the cell, the choice of encapsulation, panel framing and other ancillary installation components were found to have a larger influence than the cell in many cases. It becomes evident that broad consideration must be given to fully installed PV systems if they are to be compared.

- *What are the environmental impacts in the life cycle of III-V/silicon tandem PV modules compared to conventional silicon modules and what are the key opportunities for improvement?*

Chapter 3 developed an LCA model of the III-V/Si with a high granularity representation of the manufacturing processes and synthesis methods for all precursors in the III-V supply chain. The contribution analysis clearly highlighted the MOVPE power consumption and the silicon materials in the bottom cell as the most relevant contributors. From an LCA perspective, toxicity concerns regarding direct emissions of III-V materials during manufacturing and waste treatment do not appear to be relevant compared to the toxic emissions of fossil-based electricity generation. Thus, MOVPE power consumption is more relevant to toxic releases than the arsenic content of the III-V top cells. Evidently, reduction of power consumption during MOVPE is the most effective way to reduce most types of impacts. Alternatively, shifting background energy mixes to more renewable sources would greatly benefit PV deployment by making more advanced technologies such as III-V more competitive from an environmental standpoint.

- *How can unresolved technological pathways in the development of III-V/silicon tandem modules be incorporated in environmental assessments?*

Chapter 4 built on the experience obtained in developing an LCA model and addressed one of the main challenges/sources of uncertainty encountered: the numerous pathways (resulting from all possible design choices) that the technology could take as it evolved through its Technology Readiness Level (TRL) journey. The proposed solution was to combine all possible pathways in a single product system, represented by the corresponding (groups of) unit process(es) which would be triggered stochastically according to their chances of success. The realization that uncertainties of a very different nature than the ones usually accounted for in LCA (e.g., in flow quantities) can also be parametrized and jointly propagated revealed the potential of combined uncertainty analysis and global sensitivity analysis to deal with the numerous and diverse types of uncertainty encountered in *ex-ante*/prospective assessments. This was then picked up and fully developed in Chapter 6.

- *What are the potential ecological risks introduced by III-V/silicon tandem modules throughout their life cycles?*

Chapter 5 is developed following the realization that numerous cause-effect chains must be considered to link adoption of a technology with environmental outcomes, and that there will be equally numerous uncertainties. An LCA model calculates numerous indicators for a fixed unitary demand (the functional unit). Risk assessment models calculate endpoint indicators for a given emission. A gap needs to be filled to connect technological uptake with actual emissions. This is achieved by integrating PV demand scenarios at different spatial scales with a risk assessment model for emissions in the life cycle of the III-V/Si panels manufactured, installed and discarded in these scenarios. Time is also an important consideration, given the delayed migration of metals and metalloids in the environment (typically in the order of tens or hundreds of years). The only way to appropriately answer this question in a prospective way was to develop a fully integrated probabilistic and dynamic demand-emissions-fate model. Such a model is unprecedented for emerging PV technologies (and other consumer technologies as far as we are aware). Within each scale, a very wide spectrum of possibilities was considered, represented in more than one-hundred uncertain/variable parameters describing processes in the emissions and fate modelling during all relevant life cycle stages.

- *How can uncertainty analysis and global sensitivity analysis be used to prioritize research directions towards safer and more sustainable design of III-V/silicon tandem technologies?*

The probabilistic framework that gradually emerged from the previous chapters and took full shape in Chapter 6 is largely based on combined uncertainty analysis and global sensitivity analysis. This powerful combination provides solutions at different levels for the data limitations and concomitant uncertainty issues in the *ex-ante* problem. First and foremost, it fully reveals the uncertainties by characterizing them in a systematic and cohesive way, making any ensuing investigations/discussions more transparent. Second, it prevents the modelling effort from shying away from greater resolution or more complex representation of cause-effect chains in fear of missing data. Third, it allows focusing on the most relevant uncertain factors for refining further research: a valuable recourse given the time and resource constraints already discussed. This is in essence the so-called factor fixing for model simplification described by Saltelli et al.[8]. Here we stress that, in contrast to strategy (b) of Section 7.1, models are simplified in a way that does not significantly affect the outcomes of interest (e.g., risk or impact indicators), rather than in an arbitrary or ad-hoc manner with no prior knowledge of factor importance. Finally, but no less importantly, experience proved the framework equally useful in facilitating communication between stakeholders with very different backgrounds and different ways of understanding and dealing with uncertainties in their own domain expertise.

As a result, over a four-year period, the studied III-V/Si technology evolved from a highly undetermined system to a system with reduced uncertainty and a much better outlook regarding environmental performance. These are perhaps the two most important outcomes that can be achieved with an early-stage assessment. Throughout the course of the III-V/Si case study, concrete design choices such as laser-sintered copper metallization over other alternatives shifted the indicators of interest (e.g., LCA impact scores, risk quotients) significantly in the desired direction. Moreover, application of the framework revealed the boundary where additional design improvements by technology developers reach their effectiveness limits, i.e. diminishing returns. At this point, efforts from other actors in the technology's value chain such as consumers and end-of-life service providers can have a larger positive influence on the environmental performance of the technological system.

7.3. Limitations and future research directions

A limitation of this work is that the methods used were developed in parallel to the R&D program for the III-V/Si technology which was ongoing[9]. This meant that not all the right questions were asked to key stakeholders such as technology developers and other relevant actors in the supply chain from the beginning. It also meant that several aspects of the III-V/Si technological system were not fully fitted to the framework, even though they would have provided ideal testing grounds. Such is the case of probability distributions of technological parameters used in the models, which could have been obtained from more structured expert elicitation protocols as suggested in Chapter 6. The opportunity is now ripe to apply the framework from the beginning of an R&D program to fully demonstrate its strength.

Another limitation is that substantial interdisciplinary work is required to build and apply the underlying models. This knowledge may not always be available and will likely go beyond that of a single LCA or Risk Assessment practitioner. A close collaboration between practictioners and technology developers starting from the lower TRL levels is very beneficial (if not a necessity) in this respect, and is largely what made this III-V/Si PV case study possible. It must also be reckoned that the time invested in the III-V/Si LCA and risk assessments here presented was more than would be available for typical R&D projects. However, this included considerable time invested in methods development and this work has provided an important step forward by integrating concepts and developing software tools that can easily be adapted to case studies from other technological domains. This greatly reduces the amount of research that will be required for new case studies, allowing practitioners to focus much more on the specifics of their technology.

Additional work can be done in this front to further facilitate implementation by modellers and minimize coding requirements, e.g., using *Shiny* interfaces for the *R* scripts and improving the coupling of macro-enabled Microsoft Excel spreadsheets with R in the probabilistic dynamic risk assessment model of Chapter 5. On the LCA side, recently published work[10] associated to this thesis developed algorithms and a. user interface for applying the GSA methods proposed in Chapter 4 in a much more efficient way, but there is still room for improvement on visualization and interpretation of the GSA results.

Further work can also be done to strengthen the conceptual power and applicability of the framework. New case studies can help to demonstrate the applicability of Bayesian probabilities and expert elicitation protocols which can fully incorporate all kinds of scarce and diverse data that becomes available. Subsequent iterations of the assessments as the technology advances from low TRL to market-readiness may provide opportunities to conduct Bayesian inference which would make parameter estimation more robust. This can also lead to greater consensus amongst experts in elicitation processes. This framework may also serve as a bridge to machine learning, although the importance of model over data must be stressed. Machine learning is reliant on data and produces data rather than explanations. To guide safe and sustainable innovation, explanations are needed. That is, we need to understand the factors that matter in the technological system (and beyond), their relationships, how they can be influenced and how their changes reflect on different environmental impact and risk indicators.

7.4.Policy and societal implications

The story of a research & development (R&D) program is a story about uncertainty. While uncertainty may be uncomfortable -*an inconvenience*- for modelers, technology developers, decision-makers and their stakeholders, it is an unavoidable and central aspect of innovation. Yet we must not allow it to be paralysing. This work offers an upside to the 'inconvenience' in that it can be an important source of opportunities for safer and more sustainable designs. A deep body of work has already been developed to analyse uncertainty in natural sciences as well as finance, economics and engineering. Very sophisticated methods, more recently including machine learning and artificial intelligence, are now being introduced in these fields, helping the technological and economic dimensions of technology advance at ever larger strides. Safety and sustainability assessment cannot fall behind; if anything, it must stay ahead.

Of course, there is an underlying call for non-technical audiences -especially key decisionmakers and policymakers- to become more comfortable with the language of uncertainty *and* (global!) sensitivity. At the same time, our technical assessments must be better at interpreting and communicating these aspects. But the key message that emerges from this work is that existing uncertainties -about both positive and negative outcomes- must compel us to find a right balance between avoiding risks and hindering technological development that could have otherwise offered unforeseen societal benefits.

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