



Enabling Safe & Sustainable Innovation

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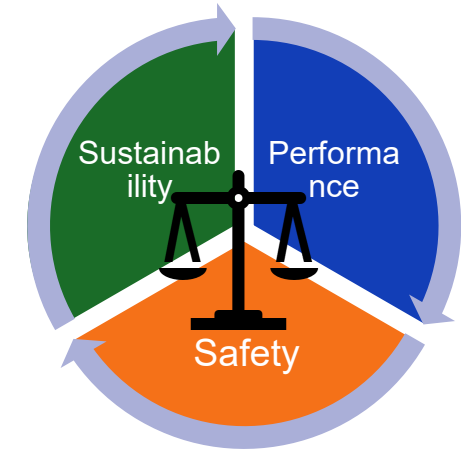
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Challenge

SSbD decision making based on trade-offs

- Multidisciplinary: costs, regulations, scientific and engineering expertise, manufacturing, sales, service, safety, sustainability.
- System and organizational complexity results into difficulties in understanding, connecting and aligning all concerns.
- Satisfying all expectations at the same time is often impossible.
- So, **Trade-offs and dilemmas** have to be addressed, which requires involvement of all stakeholders.



TNO's SSbD ambition

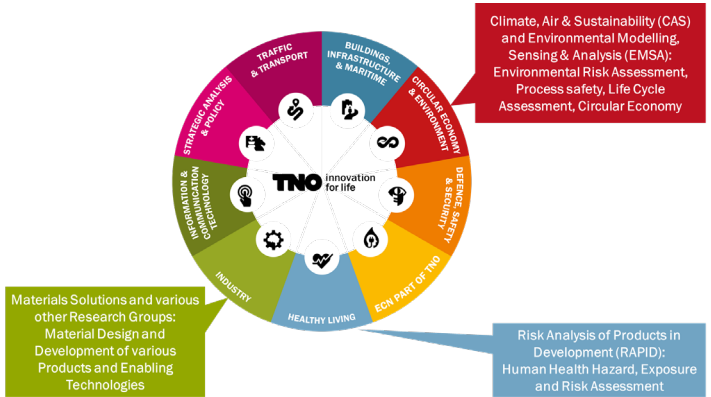
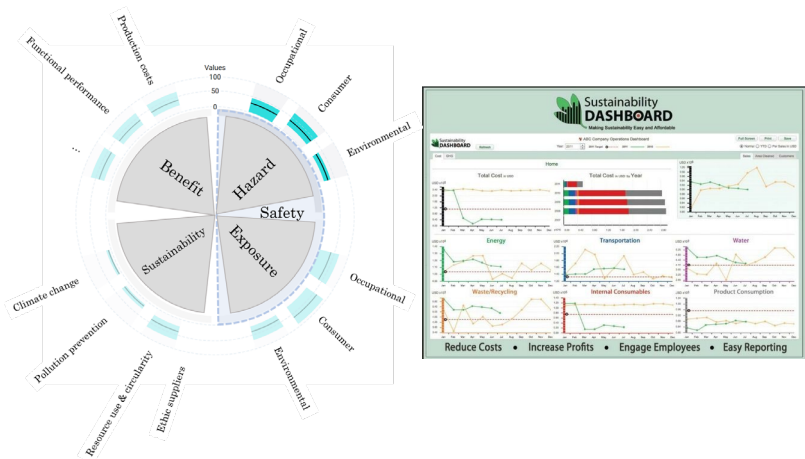
Develop a decision support system that assists industry in safe and sustainable innovation of chemicals, materials and technologies at a competitive speed

- Integrate safety, sustainability, criticality, and performance at an early stage of innovation
- Increasing chances of successful market launch

Data-driven risk-informed decision making platform

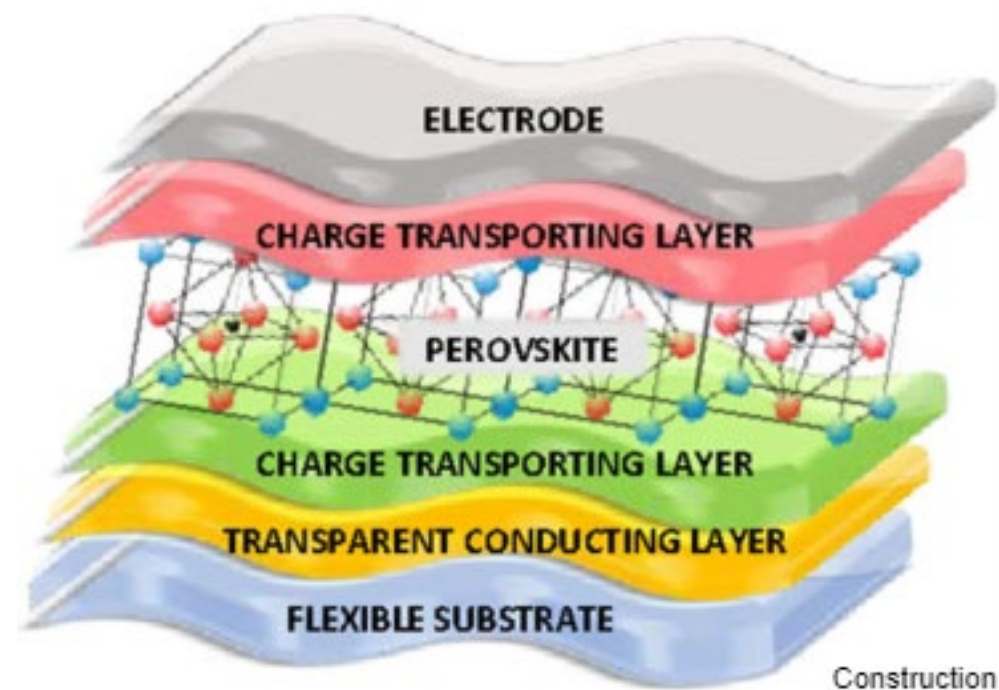
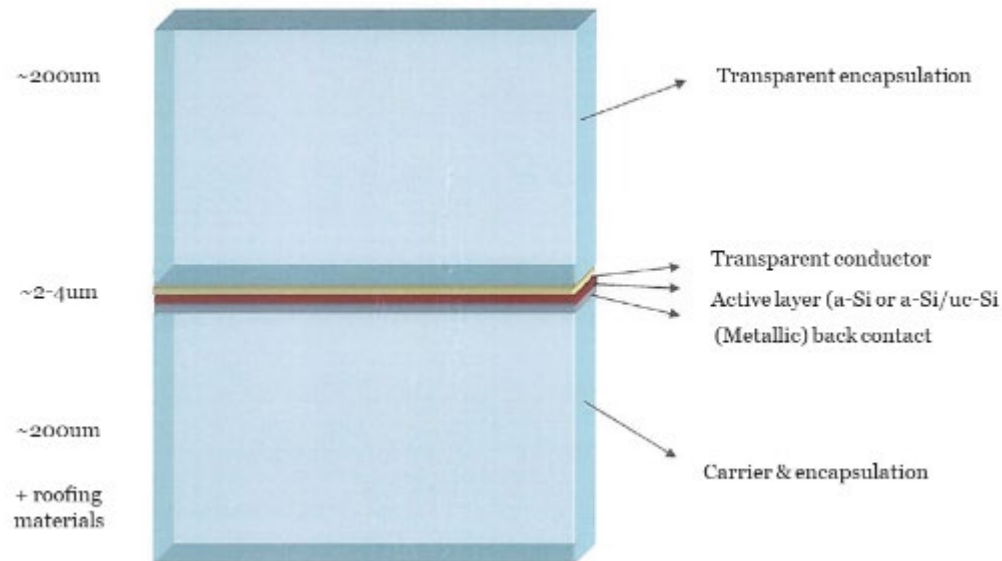
Multi-stakeholder involvement (companies, regulators, consumers)

Transdisciplinary system thinking approach



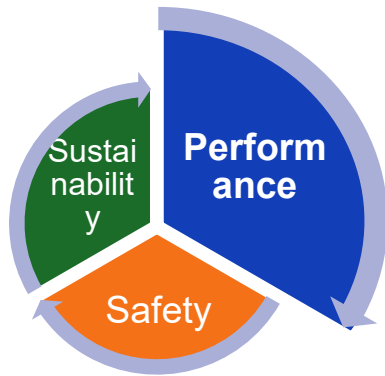
Case study: thin film solar modules

Comparing tandem α -Si/ μ -Si with single-junction perovskite thin film

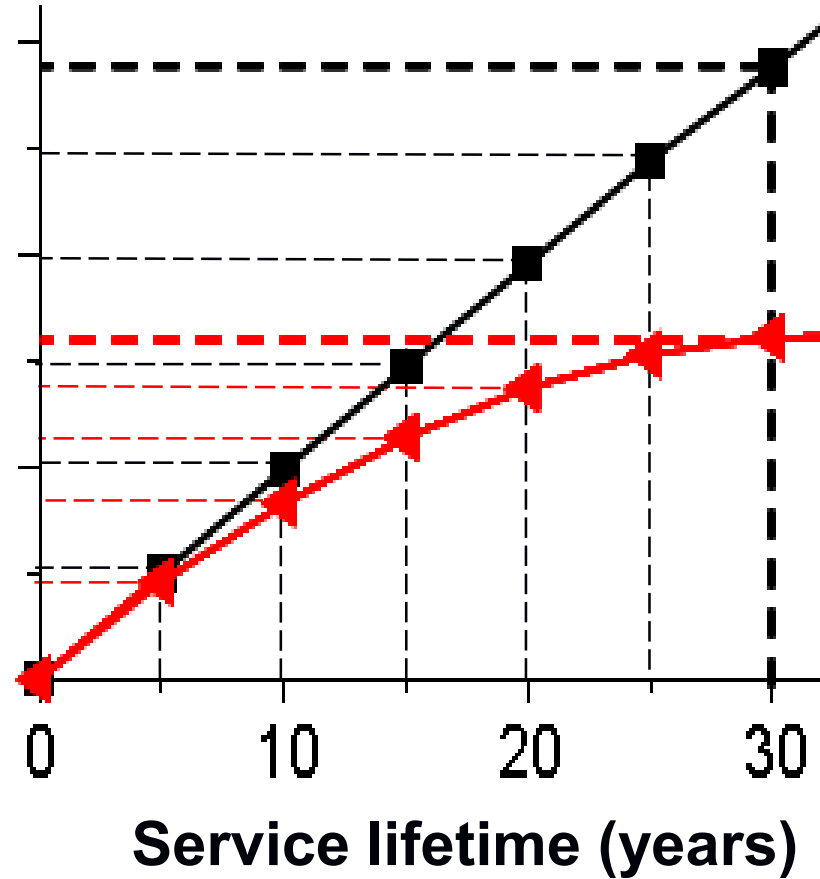


Performance

- > High efficiency
- > Low degradation rate (DR)
- > High service lifetime



Electricity generation (kWh)
cumulative throughout service lifetime

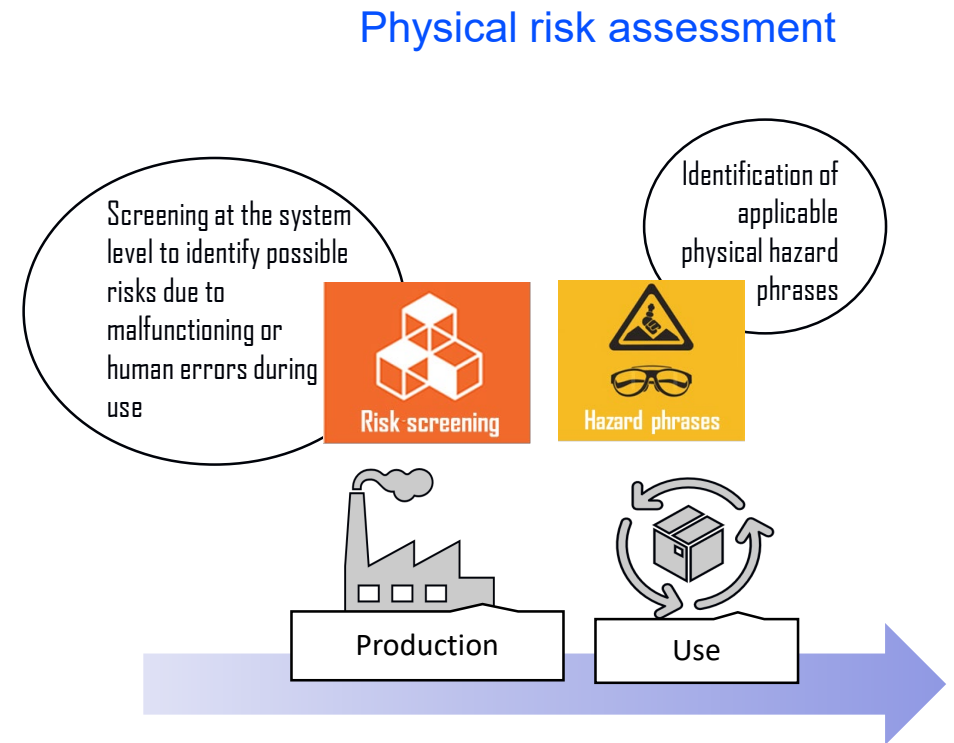
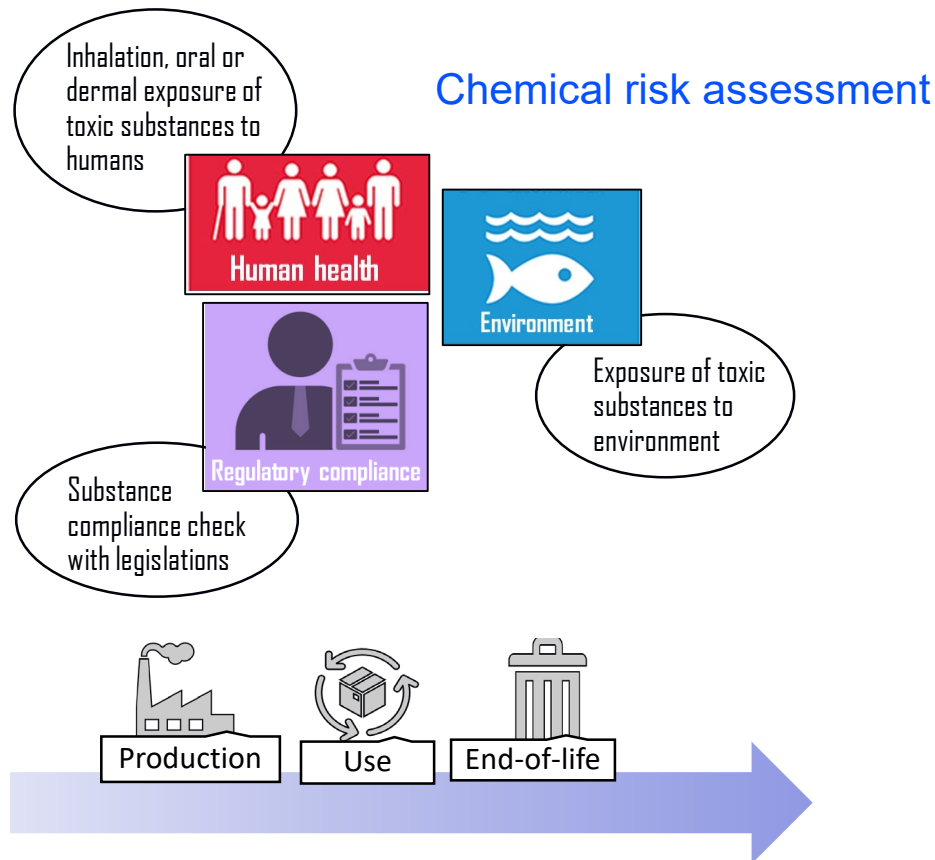


—■— 0,25% DR
—▲— 3,00% DR

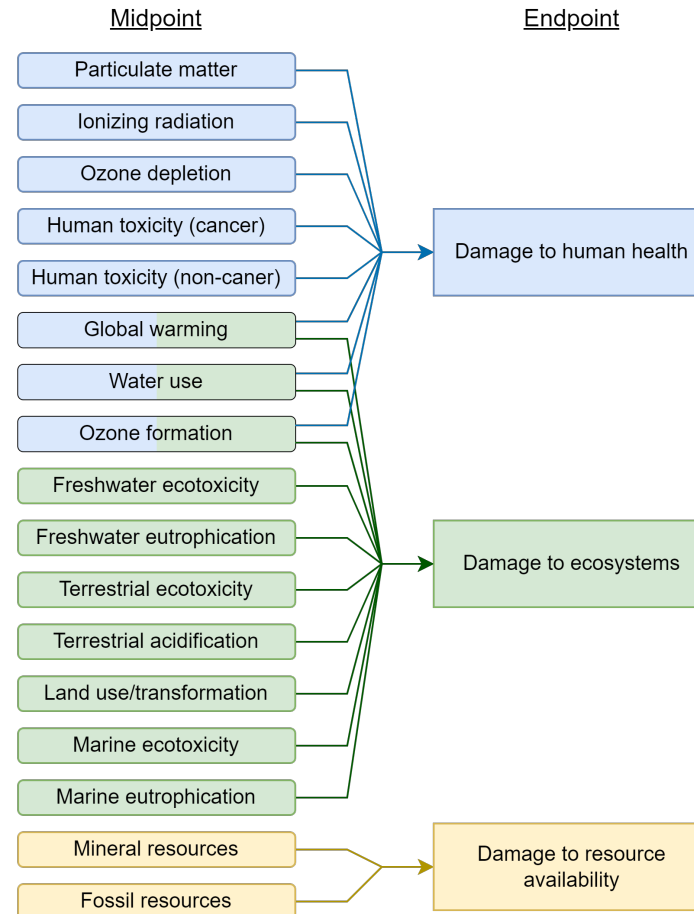
Safety



Assessment of the nature and probability of adverse health effects in humans and environmental species who get exposed to toxic substances



Life Cycle Assessment (LCA)

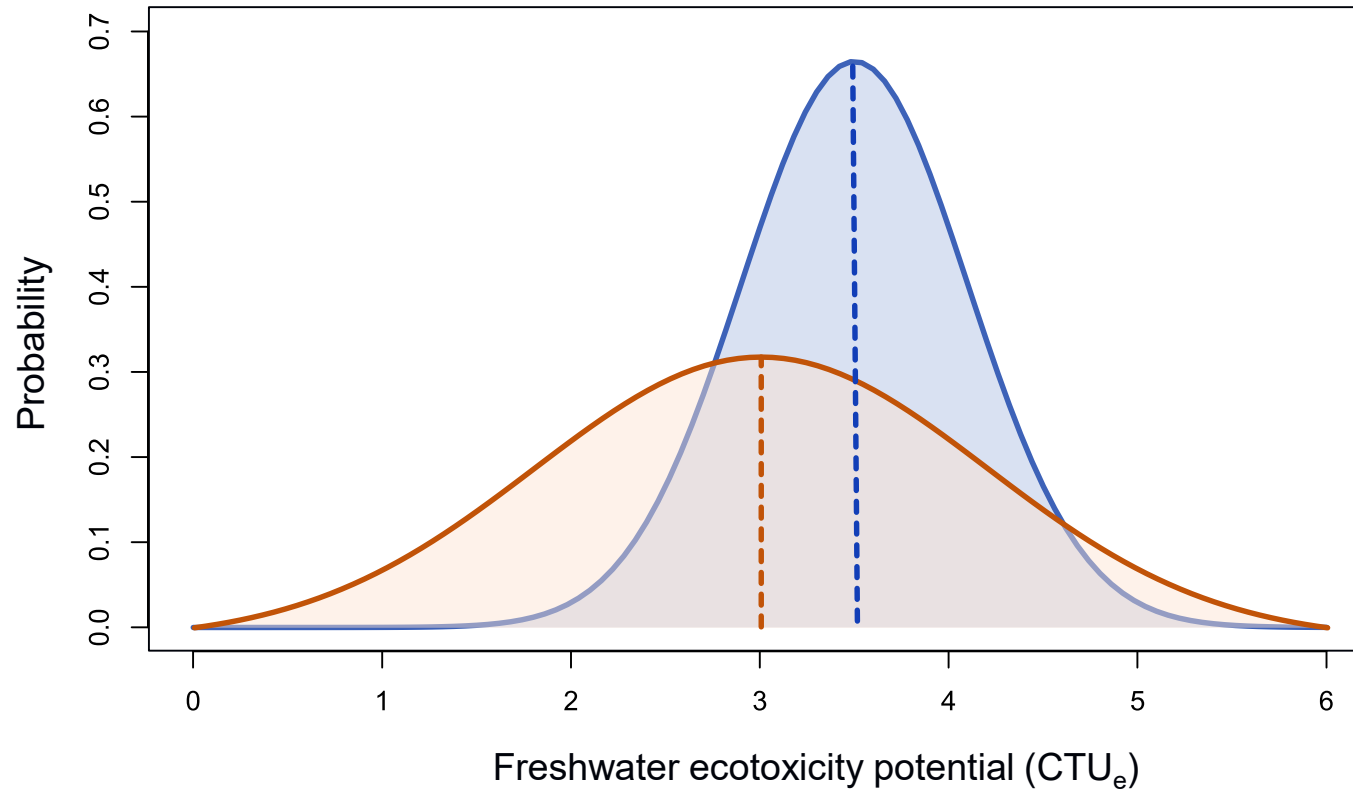


What kinds of decisions?

- Choice between different indicators, different domains
 - Ozone depletion vs. cost
- Choice between different indicators, same domain
 - Ozone depletion vs. climate change
- Choice between same type of indicator, different principle
 - Chemical risk vs. LCA toxicity indicators
- Choice between same indicator, different (quantifiable) uncertainty
 - 3 kg CO₂eq (SD: 2.0) vs. 3.2 kg CO₂eq (SD: 1.1)
- Choice between same indicator, different (unquantifiable) uncertainty
 - Toxicity of bulk material vs. toxicity of nano material
- Choice of benchmark
 - Incumbent technology vs. planetary boundaries
- Choice between same impact, different outcome for different stakeholders
 - (costs for value chain actor 1 vs value chain actor 2)
- ...other?

What kinds of decisions?

- The “two-moment decision model” (same indicator, different quantifiable uncertainty)



What kinds of decisions?

- Uncertainty and variability in USEtox characterisation factors

$$CF = FF \times XF \times EfF$$

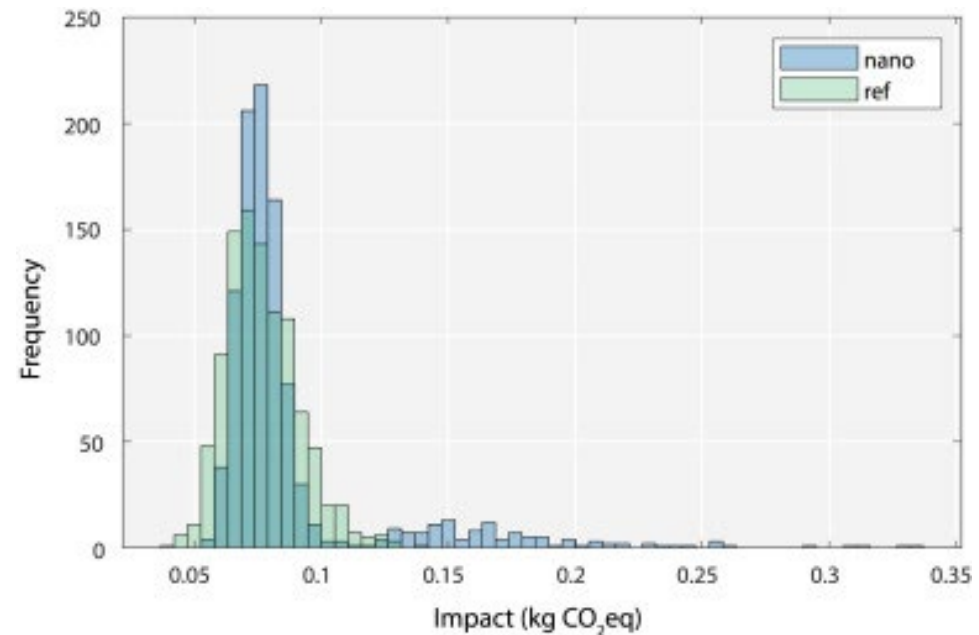
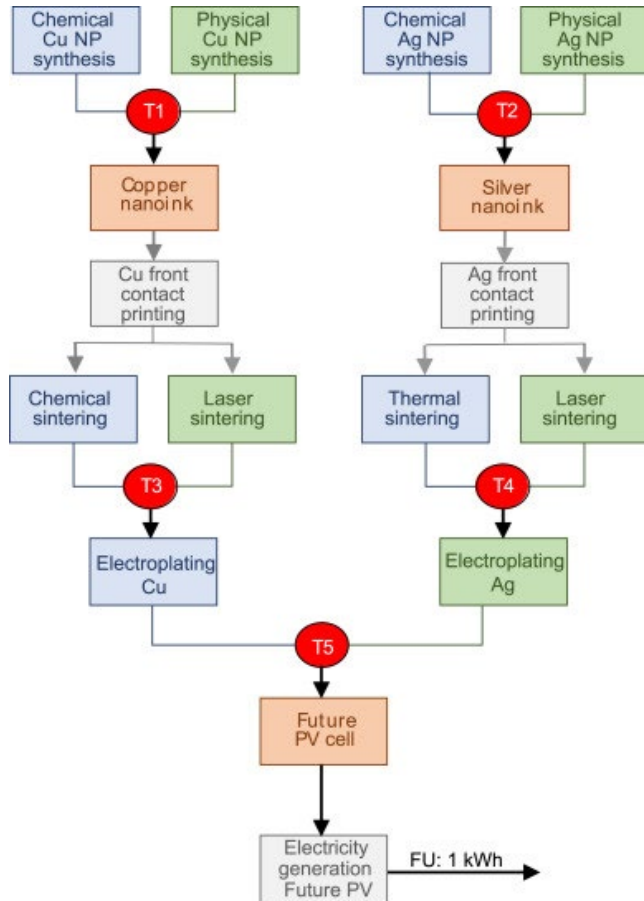
On data for EfF: “When toxicity data for at least two species were available, the HC20 was directly derived from the SSD curve (chronic EC10). However, the fewer data the lower the reliability. In fact, **uncertainty is estimated to be of 4 orders of magnitude** when only two species are available” (*Van Zelm et al. 2007, in Sala et al., 2022*).

On variability in FF: “the Kd values **can vary over several orders of magnitude for a given metal** as a function of soil properties...” (*Allison & Allison, 2005 in Groenenberg, 2011*)

On overall model uncertainty of USEtox: “...**3 orders of magnitude uncertainty on the individual factors** (...) means that contributions of 1%, 5% or 90% to the total toxicity score can be interpreted as essentially equal, but significantly larger than those of a chemical contributing to less than 1 per thousand or less than 1 per million of the total score” (*Fantke et al., 2017*)

Towards a solution

- Introducing (design) choices in underlying (LCA) models



Blanco et al., 2020. Assessing the sustainability of emerging technologies: A probabilistic LCA method applied to advanced photovoltaics. *J. Cl. Prod.*

Towards a solution

- Understanding the SSbD relevance (sensitivity) of choices

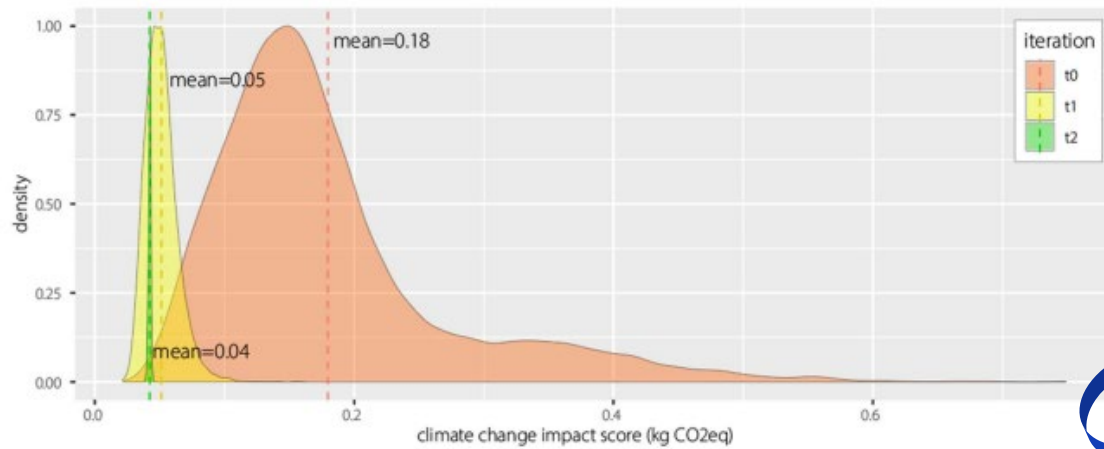


Figure 3 Probability distribution for climate change impact scores of the emerging III-V/Si technology in three successive snapshots in time: t0=initial, before the start of R&D project, t1=after R&D project, and t2=optimized roadmap for the technology

Blanco et al., (in review). A framework for guiding Safe and Sustainable-by-Design innovation. *J. Ind. Ecol.*

Cucurachi, et al., 2022. Implementation of uncertainty analysis and moment-independent global sensitivity analysis for full-scale life cycle assessment models. *J. Ind. Ecol.*

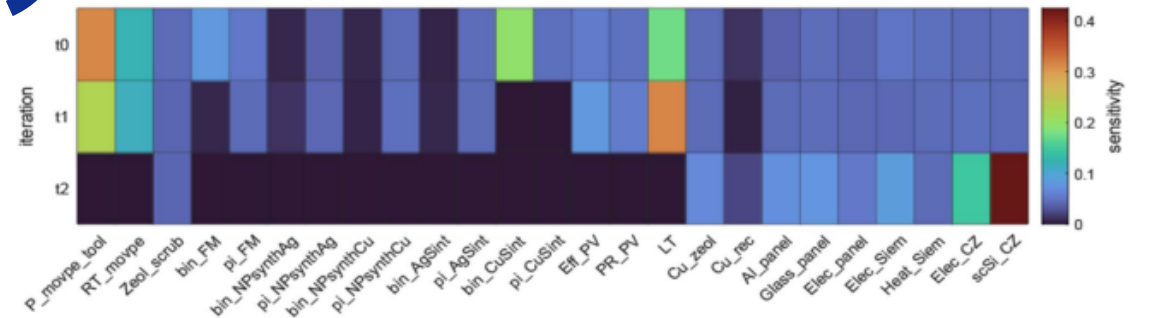


Figure 4 Delta sensitivity measures (relative to other factors) in three successive iterations: t0=initial, before the start of R&D project, t1=after R&D project, and t2=optimized roadmap for a market-ready technology. The description of each factor is provided in Table 6-2

Towards a solution

- Understanding the SSbD relevance (sensitivity) of **all** choices

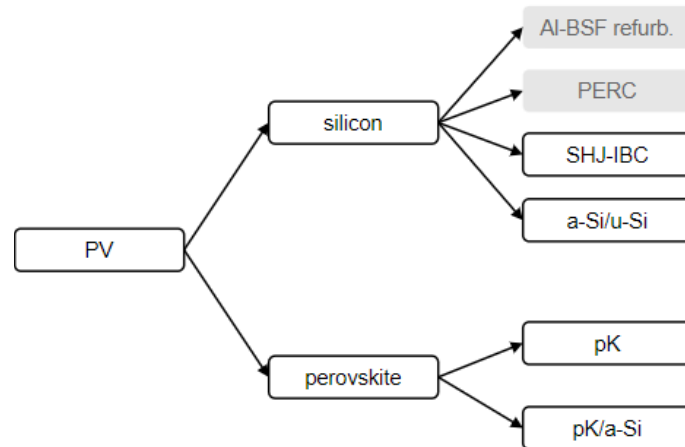


Table 2. Overview of design parameters for the prospective scenario cell designs. The abbreviations of the design names refer to the discussion of these designs in Section 2.1 and are also shown in Fig. 3, Fig. 4.

Short name	Ref-cSi	Ref-SHJ	PVD-SHJ	NE-SHJ	ALD-SHJ	IBC-SHJ
Wafer type	p-type	n-type	n-type	n-type	n-type	n-type
Wafer thickness	100	100	100	100	100	100
Passivation		a-Si:H (i)	a-Si:H (i)	a-Si:H (i)	Al2O3	a-Si:H (i)
Emitter	diffused n-dopant	a-Si:H (p)	a-Si:H (p)	multifunctional layer	ZnO	a-Si:H (p)
TCO	-	ZnO	ZnO	ZnO	ZnO	ZnO
Metallization front	Cu print	Cu plate	Cu plate	Cu plate	Cu plate	-
Metallization back	Al print with Cu soldering pads	Cu plate	Cu PVD	Cu plate	Cu plate	Cu plate
Cell area (cm ²)	239	239	239	239	239	239
Cell efficiency ^a	20.7%	25.4%	25.3%	23.2%	23.0%	25.9%
Module efficiency ^a	19.7%	24.1%	24.0%	22.1%	21.8%	24.6%

Louwen et al., 2016

Towards a solution

- Finding the set of optimal solutions: a multi-objective optimisation (MOO) approach

- Objective functions

$$CC = f(C_1, C_2, \dots)$$

$$HTP = f(C_1, C_2, \dots)$$

$$LCC = f(C_1, C_2, \dots)$$

...

C1,
C2...
Relevant
design
choices
(GSA
ranked)

- Constraints

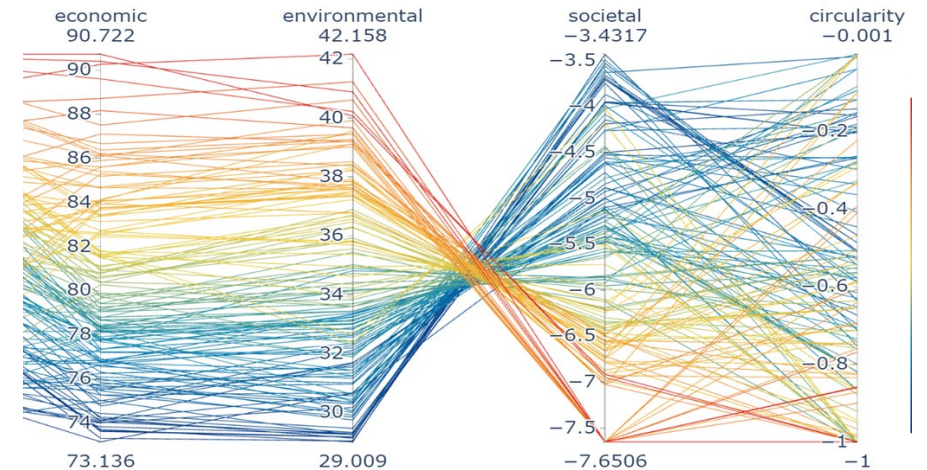
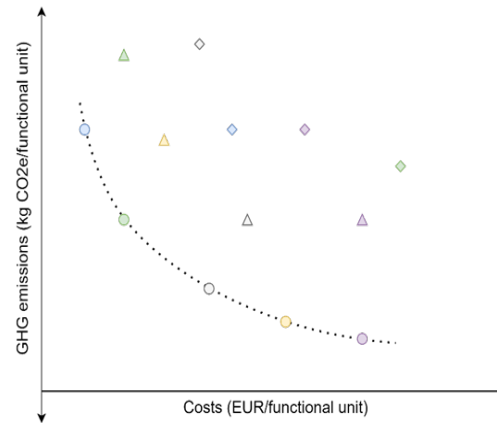
$$\text{Cost} / \text{FU}_{\text{NOV}} \leq \text{Cost} / \text{FU}_{\text{INC}}$$

$$\text{PEC}_{\text{SOIL}} \leq \text{Regulatory threshold}$$

$$\text{Material use} < \% \text{ global reserves}$$

$$\text{Children in employment} \leq 0$$

...



Source: ERP Circular Structures Project (TNO)

Towards a solution

- Deciding between the optimal solutions
 - Learnings from TNO's Circular Structures Early Research Project:

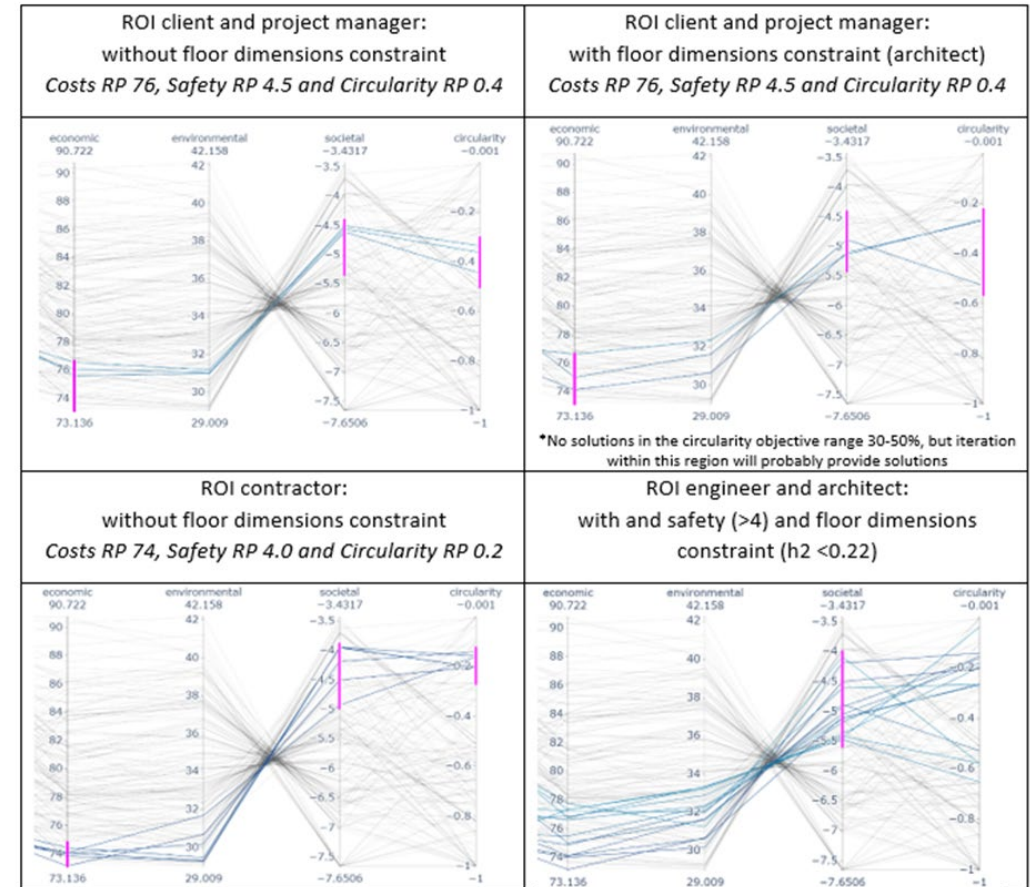


In the last years, the use cases show us that material-driven multi-criteria design optimisation tool has great potential to support decision making because it enables transparency in interdependencies of objectives thanks to the multitude of solutions and it can be implemented in an interactive multi-phase process



THE CHALLENGE is now how to test and illustrate this potential in a multi-actor decision making setting and how to guide a process to go from a multitude of pareto-optimal solutions towards one solution that suits all actors

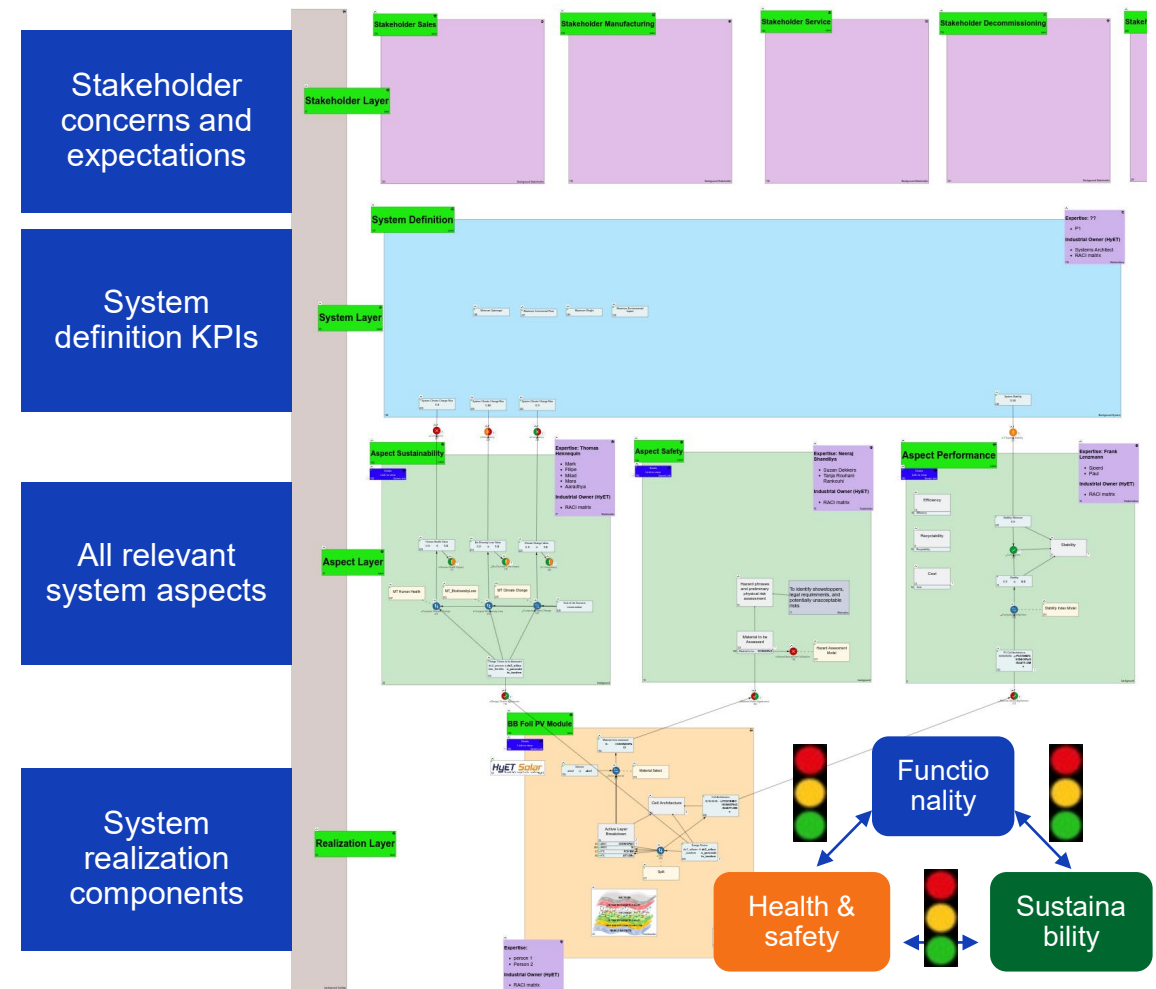
Step 4: evaluate ROI



Source: ERP Circular Structures Project (TNO)

Towards a solution

- Deciding between the optimal solutions: The DAARIUS framework
 - Qualitative & quantitative parametric reasoning and decision support framework
 - A typical reasoning configuration may include up to 20 stakeholders, 40 system defined parameters, 20 aspects and 20 system realization components.
 - All domains have connection links with "validations". These validations have colors, representing the colors of traffic lights. The color determines the alignment on the specific parameter.
 - Parameters are coupled, using "Transformations" which are built on computational models. Models can be very simple mathematical models or very complex simulations, LCAs or Safety Hazard analysis.
 - Expected tensions, e.g. performance vs. cost, which might affect the market acceptance.
 - The framework itself does not take the decisions but allows the organization to have an overall insight by exploring various design alternatives.
 - Decisionmakers can assess these scenarios and finally, the preferred scenario can be chosen.
 - This approach enables transparency to all involved stakeholders



Key messages

- Uncertainty is the substrate on which innovation lives & grows!
- A framework to support safe & sustainable innovation should embrace it, not try to work around it
- SSbD presents an archetypical post-normal science situation
 - “facts are uncertain, values in dispute, stakes high and decisions urgent”
- We need robust approaches → to identify, characterize & quantify uncertainty
- But palatable ways for diverse stakeholders to interpret, communicate, decide, reach consensus, prioritize



Does this holy grail exist?

TNO SSbD (seed) Early Research Project team

- Hedwig Braakhuis
- Wouter Fransman
- Wouter Tabingh Suermondt
- Neeraj Shandilya
- Frank Lenzmann
- Ruby Vermoolen
- Max Hennekes
- Susan Dekkers
- Thomas Hennequin
- Aaradhya Bansal
- Carlos Felipe Blanco
- Mark Huijbregts
- Mara Hauck
- Milad Golkaram

A woman with long, wavy brown hair, wearing a light purple knitted sweater, stands in a field of tall, golden-brown grass. She is holding a small, white, three-bladed wind turbine model in her right hand, extending it towards the sky. The background shows a dark ocean under a dramatic, cloudy sky. The overall mood is one of appreciation and hope for sustainable energy.

Thank you!