Framework for metamodel-driven integration of life cycle assessment and agent-based modeling

Fuortes, Agnese; Blanco Rocha, Carlos Felipe; Quik, Joris T.K.; de Jager, Lynn; Peijnenburg, Willie

DOI
10.1016/j.spc.2025.06.005

Publication date
2025

Document Version
Final published version

Published in
Sustainable Production and Consumption

Sustainable Production and Consumption 58 (2025) 14–29

Contents lists available at ScienceDirect

Sustainable Production and Consumption

journal homepage: www.elsevier.com/locate/spc

Framework for metamodel-driven integration of life cycle assessment and agent-based modeling

Agnese Fuortes [a,b,*], Carlos Felipe Blanco Rocha [b,c], Joris T.K. Quik [a], Lynn de Jager [a,d], Willie Peijnenburg [b,e]

[a] National Institute for Public Health and the Environment (RIVM), Center for Sustainability, Environment and Health (DMG), Antonie van Leeuwenhoeklaan 9, 3721 MA Bilthoven, the Netherlands

[b] Leiden University, Institute of Environmental Sciences, Einsteinweg 2, 2333 CC Leiden, the Netherlands.

[c] Netherlands Organisation for Applied Research (TNO), Circularity & Sustainability Impact Group, Princetonlaan 6, 3584 CB Utrecht, the Netherlands.

[d] Technical University Delft, The Faculty of Technology, Policy, and Management, Jaffalaan 5, 2628 BX Delft, the Netherlands

[e] National Institute for Public Health and the Environment (RIVM), Centre for Safety of Substances and Products (VSP), Antonie van Leeuwenhoeklaan 9, 3721 MA Bilthoven, the Netherlands

ARTICLE INFO

Editor: Dr. Carlos Pozo

Keywords:
Agent-based modeling
Life cycle assessment
Metamodel
Coupling

ABSTRACT

The energy transition brings about complex environmental and societal changes that require robust science-based policy guidance. Conventional Life Cycle Assessment (LCA) methods to evaluate the implications of these changes often fail to capture the dynamic interactions among energy systems, human behavior, and environmental impacts, leading to potentially misleading or oversimplified conclusions. This study introduces a new framework for integrating societal change into LCA using Agent-Based Modeling (ABM). Our approach leverages LCA metamodels, integrated with the ABM via defined linking parameters, to enable real-time feedback between agent decisions and environmental outcomes, while minimizing computational demands. We illustrate the applications of this framework in a photovoltaic case study, examining how end-of-life choices affect abiotic depletion and climate change. The ABM-LCA integration employs metamodels with high predictive performance, achieving R^2 values of 0.95 for abiotic depletion and 0.82 for climate change. Linking parameters are based on the number of PV modules entering different end-of-life pathways. Societal change, as modeled in the ABM, is driven by the assumption that increased awareness of environmental impacts promotes circular behaviors. The photovoltaic case study provides an illustrative exploration of how consumer choices may affect environmental impacts, such as abiotic depletion and climate change, and how these impacts, in turn, may shape future consumer behavior. This work highlights the value of using a metamodel-driven, integrated ABM-LCA modeling framework for decision-making in complex systems, uncovering unexpected system behaviors and offering insights into sustainable transitions.

1. Introduction

The energy transition is a complex process with both positive and negative environmental and societal impacts, making it essential for decision-makers to rely on robust, science-based policy advice. While renewable energy reduces emissions, it can also lead to issues such as land-use conflicts and biodiversity loss. Producing reliable advice is challenging due to the unpredictable interactions between energy systems, infrastructure, policies, and human behaviors (Geels et al., 2017). Current forecasting and scenario models often fail by oversimplifying uncertainties and neglecting human behavior, leading to biased interpretations (Bezdek and Wendling, 2002; Carrington and Stephenson, 2018; Morgan and Keith, 2008; Scoones and Stirling, 2020; Stirling, 2010).

Integrating the dynamics of human behavior into environmental assessments offers significant benefits for understanding the complexities of the energy system. This integration allows for a better exploration of the different dimensions of uncertainty linked with system complexity, exposing the emergence of unexpected system behaviors. It also supports the development of behaviorally-informed policy advice

* Corresponding author at: National Institute for Public Health and the Environment (RIVM), Center for Sustainability, Environment and Health (DMG), Antonie van Leeuwenhoeklaan 9, 3721 MA Bilthoven, the Netherlands.

E-mail address: agnese.fuortes@rivm.nl (A. Fuortes).

https://doi.org/10.1016/j.spc.2025.06.005
Received 5 March 2025; Received in revised form 23 May 2025; Accepted 9 June 2025
Available online 11 June 2025

that moves beyond static assessment of environmental impacts and towards identifying the underlying mechanisms that govern complex systems. As a result, decision-making processes can account for the diversity of perspectives, values, and preferences in the transition towards a sustainable energy system.

Agent-Based Modeling (ABM) is increasingly recognized as a robust computational method for analyzing complex energy systems characterized by actor heterogeneity, noncentralized decision making, and system level feedback (Dam et al., 2013; Hansen et al., 2019). ABM enables the explicit representation of individual agents whose behaviors are defined by rule-based logic and evolve over time in response to endogenous and exogenous variables such as spatial constraints, social network effects, and information availability. Yet, ABM alone is often insufficient for guiding sustainability policy, as it typically lacks an explicit environmental assessment component. To address this gap, researchers have started integrating ABM with Life Cycle Assessment (LCA), a methodology defined by the International Standard Organisation (ISO) as a systematic assessment of the environmental impacts of a product system across its entire life cycle (ISO, 2016).

Existing approaches to integrating LCA and ABM typically fall into three categories. Some studies adopt a soft coupling approach, where demand scenarios generated by ABM serve as inputs for LCA calculations without real-time interactions between the models, while others use a tighter coupling strategy, feeding ABM-generated outputs into LCA at each time step of the simulation (Micolier et al., 2019; Onat et al., 2017; Zupko, 2021). Only few pioneering studies consider the influences of impacts on agents' behaviors by introducing a feedback loop, where data are exchanged between LCA and ABM at each time step, and LCA results are used as input parameters for the ABM simulation and vice versa. This approach is defined in the literature as “LCA/ABM Symbiosis” or “hard-couple” (Baustert and Benetto, 2017; Marvuglia et al., 2022; Micolier et al., 2019).

This bi-directional integration not only reveals how the behavior and decisions of consumers, policymakers, and companies influence environmental impacts but also shows how awareness of those impacts can, in turn, alter future behaviors. Despite its clear potential, this integration remains relatively uncommon in practice, due to lack of flexible and interoperable frameworks that can accommodate different types of feedback (Section 2.1). ABM and LCA models are often developed in distinct software environments and programming languages, and the absence of language agnostic frameworks to facilitate their integration introduces significant technical barriers while also potentially limiting the accessibility and replicability of such models (Micolier et al., 2019; Navarrete Gutiérrez et al., 2015). Although the agent based modeling paradigm is increasingly being explored within the life cycle assessment community, it has not yet achieved widespread acceptance, and its practical implementation remains limited, particularly for users without specialized expertise (Marvuglia et al., 2018, 2022). Comparable difficulties are likely within the ABM community, where incorporating LCA introduces unfamiliar methodological demands. As MacLeod and Nagatsu (2018) observe, interdisciplinary research often faces significant challenges in reconciling domain-specific practices, as it typically demands considerable cognitive, conceptual, and methodological restructuring. These barriers continue to impede broader implementation of integrated assessment approaches.

To overcome these methodological and interdisciplinary barriers to integration, this study proposes a modeling framework that facilitates the hard coupling of LCA and ABM through computationally efficient strategies. Central to this approach is the use of a metamodel, a simple approximation function that retains all the specifics of the original LCA model while allowing seamless integration into the ABM simulation by non-LCA specialists (Li et al., 2010). The metamodeling strategy enhances computational feasibility, promotes software interoperability, and lowers the technical barriers to adoption without sacrificing analytical rigor. As a result, it not only improves the scalability of the integrated models, allowing them to efficiently handle a growing number of agents and interactions, but also provides a flexible, modular framework that can be adapted and extended to a wide range of application domains. To demonstrate the potential of our integrated modeling approach, we apply and evaluate our framework on photovoltaics, showcasing its capability to provide deeper insights into sustainable energy transitions.

2. Literature review

2.1. ABM-LCA hard-coupling

The computational approaches to achieving hard coupling between LCA and ABM in the literature typically involve integrating dynamic agent-based simulations with static LCA databases (Bichraoui-Draper et al., 2015; Davis et al., 2009; Lan et al., 2019; Miller et al., 2013). This integration allows the evolving decisions and actions of agents, such as changes in consumption patterns, recycling behaviors, or energy use, to influence the foreground system parameters, which are then assessed using static background LCA data. Because background systems are generally assumed to be linear and unaffected by individual behavior, their impacts can be precomputed and reused across simulation steps, thereby avoiding repeated matrix inverse operations (Marvuglia et al., 2022).

Although individual LCA calculations are not inherently computationally intensive, the burden increases significantly when calculations must be repeated for each agent at every simulation step. This repetition becomes especially demanding in large-scale ABMs with fine-grained behavioral heterogeneity. Precomputing impacts is therefore a valuable and computationally efficient strategy, but only under the condition that background processes remain unaffected by the evolving dynamics of the ABM.

In addition to these computational considerations, the technical complexity of implementing such methods presents a barrier. Hard-coupled models often require detailed knowledge of both LCA methodology and its underlying mathematical structures, which can limit accessibility for interdisciplinary researchers. Despite growing interest in ABM-LCA integration, the literature still lacks a computational approach that can accommodate any type of integration including dynamic background interactions while maintaining computational efficiency and minimizing the need for LCA-specific expertise or manual reconfiguration.

Beyond computational and methodological considerations, a unified framework is needed to accommodate the heterogeneous ways in which LCA results are used to influence agent behavior across different modeling approaches. For example, in the simulation by Davis et al. (2009), agents are aware of the reductions in CO_2 emissions associated with their previous actions and adjust their behaviors accordingly. Miller et al. (2013) integrate life cycle inventory results from previous time steps into the decision-making process of agents, although specific criteria fed back into the ABM are not detailed. Navarrete Gutiérrez et al. (2015) implement a static feedback loop where farmer agents are given the pre-calculated LCA scores of crops at the start of the simulation, guiding their decisions without dynamic updates throughout the process. Walzberg et al. (2019) use smart meters to provide real-time electricity consumption data to inhabitants, who adjust their behaviors based on feedback on their energy usage, not an impact score. Lan et al. (2019) describe a dynamic approach where at the beginning of the year farmers decide on crop based on information received from the LCA about the potential environmental impact of each crop, whilst at the end of the year the impact from the actual decisions is calculated.

2.2. Metamodeling in LCA and ABM

The use of metamodels has become increasingly common in both LCA and ABM, particularly as a strategy to address computational burdens. In LCA, metamodels have been widely applied for uncertainty and sensitivity analysis (Jian et al., 2021; Khang et al., 2017; Li et al., 2023; Rivera and Sutherland, 2015), as well as for optimization and predictive tasks (Akhshik et al., 2022; Dabbaghi et al., 2021; Karamian et al., 2023; Polo-Mendoza et al., 2023; Shekoohiyan et al., 2023).

In the ABM literature, metamodeling has likewise emerged as a valuable methodological extension, supporting sensitivity analysis (Ligmann-Zielinska et al., 2020; Parry et al., 2013; ten Broeke et al., 2021; Thiele et al., 2014; Walzberg et al., 2021), calibration (Lamperti et al., 2018), and empirical validation (Barde and van der Hoog, 2017). Additionally, metamodels have been used to derive bifurcation diagrams, offering insights into system resilience and stability (Van Strien et al., 2019).

Although integration across modeling paradigms remains relatively rare, one example is the work of Papadopoulos and Azar (2016), who employed a surrogate function to link an ABM with a building performance simulation, enabling dynamic feedback between occupant behavior and energy use. This illustrates how metamodels can, in some cases, support interaction between distinct modeling frameworks beyond their role in computational simplification.

3. Methods

3.1. Framework integrating LCA and ABM

While the framework has been developed in the context of integrating ABM with LCA (Fig. 1), the same methodology can be applied to integrate ABM with any type of impact assessment model.

The first step involves collecting and harmonizing the necessary data for each model ensuring that consistent datasets are applied uniformly across the models to maintain coherence and accuracy throughout the framework. For LCA, this includes inventory data on material and energy inputs, emissions, and resource use. For ABM, data encompasses agent behaviors, interactions, and decision-making rules within the system and techno-economic factors such as costs, market prices, and economic and technological constraints. For data points characterized by uncertainty and variability, relevant probability distributions are compiled.

The second step involves the implementation of the metamodel. First, we identify variable/uncertain parameters that are shared by both models, henceforth called “linking parameters”. These parameters could include factors such as initial product demand, use behavior (e.g., consumption quantities and maintenance frequency), end-of-life pathways, as well as any factor that could be the outcome of the decision making of agents in the ABM and be relevant for the LCA. These parameters are assigned uniform probability distributions to capture the entire range of possible values and outcomes, avoiding any bias towards specific, likely values. This approach ensures an unbiased exploration of the parameter space, capturing a broad spectrum of potential scenarios.

Next, the parameterized LCA is implemented and run stochastically with these initial parameters, accounting for variability and uncertainty to produce a range of potential outcomes. The stochastic inputs and outputs are used to construct a metamodel, a simplified function capable

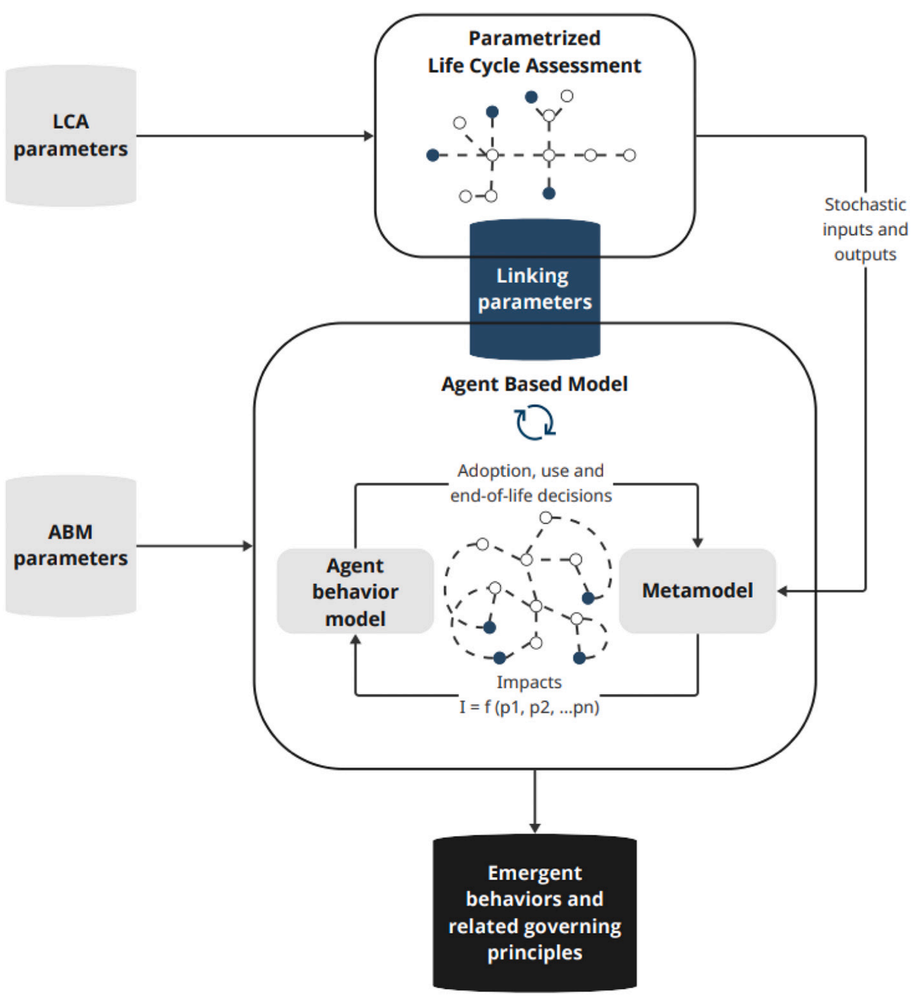

Fig. 1. Conceptual framework for integrating ABM and LCA using a metamodel approach. The metamodel approximates environmental impacts (I) as a function of a defined set of variable or uncertain parameters (p_1, p_2, …, p_n).

of approximating the results of the more complex LCA. At this stage, sensitivity analysis, which is a byproduct of the metamodel development, helps to evaluate the degree to which human behavior can influence environmental impacts, thereby validating the selection of linking parameters and the relevance of the integration from an LCA perspective (Hicks, 2022). Evaluating how environmental impacts influence human behavior, however, requires applying available behavioral theories, tailored ad hoc for the specific case study. The third step involves the linking of the ABM and LCA.

The metamodel function is then integrated into the ABM code, enabling the real-time analysis of the 2-way relationship between agents' decisions and impacts during the ABM simulations. Finally, the ABM is run stochastically and analyzed to gather insights into possible emergent behaviors and tipping points within the system, helping identify the governing principles of these behaviors and offering valuable information for decision-making.

3.2. *Case study: step 1 data alignment and harmonization*

Our case study is based on two pre-existent models: a LCA on III-V/Silicon photovoltaic (PV) panels and an ABM on end-of-life crystalline silicon (c-Si) PV panels (Blanco et al., 2020a; Blanco et al., 2025; Walzberg et al., 2021). Since these models were not developed from scratch for this study, harmonization of the data and scope was conducted post hoc to ensure compatibility.

First, we aligned the system boundaries, by expanding the LCA to include the end-of-life (EoL) phase. Then, we adjusted the geographical location of the use phase of the LCA and added transport to adapt to the US setting of the ABM case study. We also addressed differences in the solar technologies analyzed in the two papers, particularly in terms of material composition. For this study, we focused on the LCA's emerging PV technology that employs III-V semiconductor materials, such as Indium and Gallium, which are critical raw materials. While III-V technology promises efficiency improvements, it also involves trade-offs by relying on scarce materials, contributing to material depletion impacts. Thus, efficient use and recovery of these materials are critical to mitigating abiotic depletion.

These adaptations allowed us to integrate existing models into our case study, providing a practical demonstration of the proposed framework while yielding meaningful insights from both environmental and circularity perspectives.

3.2.1. *Agent based model*

Walzberg et al. (2021) analyzed the EoL fate of C-Si panels in the US over a 30-year period. The model evaluates five EoL strategies: repair, reuse, recycling, landfilling, and storage, and includes scenarios for purchasing both new and used PV panels. Furthermore, it incorporates four types of agents: PV owners, manufacturers, installers, and recyclers, and each agent type operates under specific behavioral rules, making the model extremely sophisticated (Fig. 2).

For our analysis, we focused specifically on the portion of the model concerning PV owners. The model code was taken from https://github.com/NREL/ABSiCE (accessed: 21/11/2023). A simplified description of the model is provided in Section A2 of the Supplementary Information (SI), including comparisons between the original and integrated model versions where relevant. For comprehensive documentation and full model specifications, we refer readers to the original publication by Walzberg et al. (2021).

The ABM simulates the behavior of 1000 PV owners, whose decisions are influenced by economic, environmental, and social factors. To capture social interactions, PV owner agents are initialized in a small-world network structure, generated using the Watts–Strogatz algorithm. Agent decision-making is guided by the Theory of Planned Behavior. In this framework, choices regarding PV adoption and EoL strategies are shaped by three components: perceived behavioral control (influenced by cost), subjective norm (influenced by interaction with other agents) and attitude level towards circular pathways (pro-environmental attitude) as opposed to linear pathways.

Several components of the model incorporate stochasticity. First, the initial attributes of agents are randomly assigned. For example, attitudes towards circular EoL pathways (such as reuse or recycling) are drawn from a normal distribution with a mean of 0.544 and a standard deviation of 0.1, truncated between 0 and 1. The mean and standard deviation were calibrated to reflect observed low adoption rates of recycling and reuse in 2020. Attitudes towards adopting used PV panels are similarly assigned using a normal distribution with a mean of 0.233 and standard deviation of 0.262. Additional behavioral parameters, such as inter-agent trust, are initialized from uniform distributions, and economic variables, including resale values and costs, are drawn from triangular distributions. Second, randomness is embedded in the network itself. The construction of the social network includes a probabilistic rewiring step, which introduces heterogeneity in how agents are connected, reinforcing the model's ability to simulate diverse social contexts. Third, the model's scheduler also introduces stochasticity. At each time step, agents are activated in a random order, meaning that the sequence of decisions and interactions can vary across simulation runs. To ensure reproducibility, all stochastic components are controlled using predefined random seeds.

As part of step 1, we aligned the model with the LCA by reducing the EoL pathways to selling/reusing, recycling, and landfilling, as possible in the settings of the original model. The new rates were calculated by setting repair and storage to zero and normalizing the other rates in the interval 0–1 to keep proportions intact. Then, we added fixed recovery rate parameters for gallium and indium to the ABM to account for their presence in III-V/Si solar panels (Table 1). While no changes were made to the ABM's structure or dynamics, these parameters were incorporated to align the model with the LCA. The modified code and a detailed documentation of all changes to the original code are available (Fuortes et al., 2025).

3.2.2. *Life cycle assessment model*

The model utilized in this study is derived from the recent publication by Blanco et al. (2025), which builds on their earlier 2020 work. This model represents the life cycle of PV panels, covering their production and use phases. The functional unit, i.e. the standardized measure of the product system's performance (ISO, 2016), is defined as 1 kWh of electricity generated by a slanted-roof PV installation. This unit allows for a consistent comparison of environmental impacts relative to the amount of electricity produced. Blanco et al. (2020a) compare the environmental impacts of two designs of III-V/Si cells, developed by Fraunhofer ISE, with those of conventional c-Si panels. For our case study, we selected the specific III-V/Si cell design with a higher indium consumption in its manufacturing, i.e., the Concept B “bonding” approach. Blanco et al. (2020a) employ the impact assessment method recommended by the International Reference Life Cycle Data System (ILCD), evaluating impacts across categories such as climate change, human toxicity, freshwater ecotoxicity, ionizing radiation, and depletion of mineral and metal resources. In our case study, we focused specifically on two impact categories: abiotic depletion and climate change. Abiotic depletion was chosen due to the increasing demand for virgin gallium and indium, two critical metals vital for III-V/silicon PV technology, which raises potential long-term sustainability concerns. Climate change was included as a second impact category for comparative analysis to further test the framework.

As part of step 1, we aligned the LCA to the ABM, by including an EoL phase, allowing the panels to be reused (sold), landfilled, or recycled.[1] Given the geographical differences between the LCA for III-V Si panels in Europe and the ABM for c-Si panels in the US, we adjusted the phases of production, use, and transport by changing the location of the processes

[1] More detail on how the EoL phase in SI (Section A1).

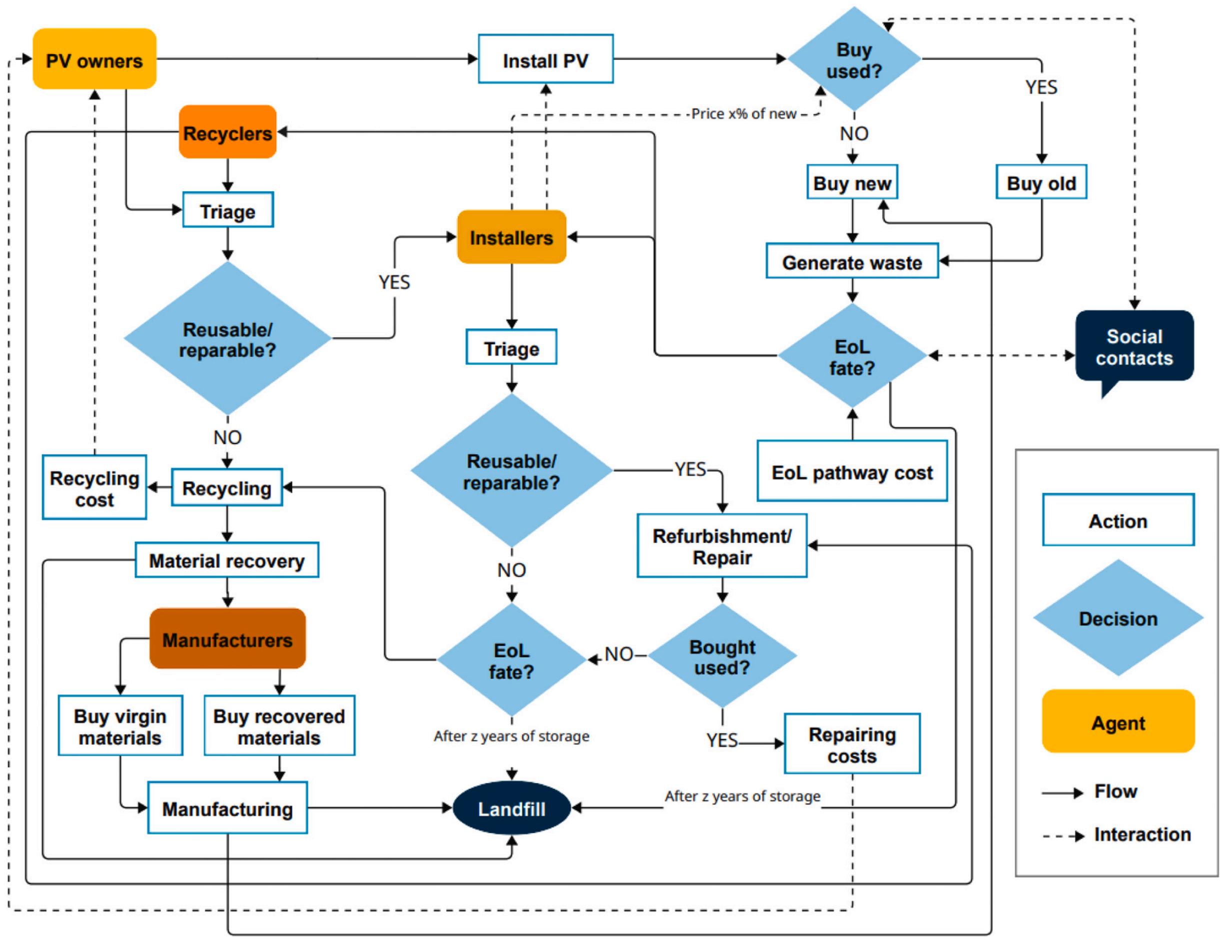

Fig. 2. Simplified schematic of the ABM, adapted from Walzberg et al. (2021).

or adding transport. We assumed the cell module production would occur in the EU and therefore maintained as in the original model with the addition of transport to allow for usage and disposal in the US. We adapted the production of the mounting system and inverter to the US context and adjusted the use phase by switching from the EU to the US energy mix.

3.3. *Case study: Step 2 implementation of the metamodel*

3.3.1. *Life cycle assessment data*

The LCA was run stochastically with 10,000 simulations, using the open-source software Activity Browser (Steubing et al., 2020), based on the Brightway2 framework (Mutel, 2017) for LCA calculations. These simulations were based solely on the uncertain foreground parameter distributions specified in Table 1. The background database remained fixed and was not sampled during the simulations.

The EoL pathways and the recycling recovery fractions are the main linking parameters[2] with the ABM, therefore they were assigned broad distributions. The other distributions, related to technological design and performance parameters, were inherited from the original LCA model of Blanco et al. (2020a) and updated according to Blanco et al. (2025).

3.3.2. *Life cycle assessment metamodel*

The stochastic inputs and outputs of the LCA model were used to generate the metamodel with the SobolGSA software (Kucherenko, 2013). We selected the Random Sampling-High Dimensional Model Representation (RS-HDMR) regression, a method for breaking down a complex function into simpler polynomial components, choosing appropriate basis functions based on input distributions, constructing an approximation function, and measuring the accuracy of this approximation (G. Li et al., 2002, 2006; Zuniga et al., 2013).

An integrable function with multiple variables $f(x) = f(x1, x2, \ldots, xn)$ can be decomposed in component functions using ANOVA-HDMR decomposition. Assuming that component functions are piecewise smooth and continuous they can be decomposed using a complete set of orthonormal polynomial basis functions (Eqs. (1) and (2)).

$$f_i(x_i) = \sum_{r=1}^{\infty} \alpha_r^i \phi_r(x_i), \quad \forall i \in \{1, 2, \ldots, n\} \tag{1}$$

$$f_{ij}(x_i, x_j) = \sum_{p=1}^{\infty} \sum_{q=1}^{\infty} \beta_{pq}^{ij} \phi_p(x_i) \phi_q(x_j), \quad \forall i < j \in \{1, 2, \ldots, n\} \tag{2}$$

For example, $\phi r(x_i)$ represents one-dimensional basis functions and $\phi pq(x_i, x_j)$ represents two-dimensional basis functions. The choice of basis functions depends on the probability distribution of the inputs. For example, for inputs uniformly distributed, Legendre polynomials are suitable.

The RS-HDMR regression method was chosen as it is generally more efficient for metamodel accuracy, achieving higher precision with the same number of sampled points (Spiessl et al., 2019). With this regression method, the coefficients of decomposition α_r^i and β_{pq}^{ij} are estimated by minimizing the mean square error of the approximation function. The approximation function $\widetilde{f}$ up to the second order of interaction can be expressed as Eq. (3).

[2] A flowchart showing the location of the parameters is provided in SI (Figure A1)

Table 1
Parameters' distributions (μ: mean, σ: standard deviation, a: minimum, b: maximum, c: mode).

Parameter name	Description	Distribution	Par-1	Par-2	Par-3
RT_movpe	MOVPE[a] runtime	Triangular	a = 0.5	b = 3.5	c = 3.5
P_movpe_tool	MOVPE tool power load per processed wafer area	Triangular	a = 1	b = 509	c = 509
Eff_PV	Cell conversion efficiency	Triangular	a = 0.25	b = 0.31	c = 0.28
PR_PV	Performance ratio	Triangular	a = 0.8	b = 0.9	c = 0.85
Cu_zeol	Scrubber granulate copper fraction	Triangular	a = 0.2	b = 0.7	c = 0.3
Al_panel	Aluminum in panel	LogNormal	μ = 0.97	σ = 0.199	–
Glass_panel	Glass in panel	LogNormal	μ = 2.31	σ = 0.199	–
Elec_panel	Electricity to manufacture panel	LogNormal	μ = 1.55	σ = 0.199	–
Zeol_scrub	Hazardous gas abatement – mass of granulate consumed per mass of gas inflow	Triangular	a = 2.55	b = 7.65	c = 7.65
LT	Lifetime of solar cell	Normal	μ = 30	σ = 5	–
Landfill_fraction	Fraction of waste going to landfill instead of recycling	Uniform[b]	min = 0	max = 0.99	–
Reuse_fraction	Fraction of EoL PV sold/reused instead of disposed of	Uniform[b]	min = 0	max = 0.99	–
Cu_rec, Al_rec, Glass_rec, Silicon_rec, Ag_rec, Ga_rec, In_rec	Recovery fraction for each material: Copper, Aluminum, Glass, Silicon, Silver, Gallium and Indium	Uniform[b]	min = 0.5	max = 0.99	–
Elec_Siem	Electricity consumption of Siemens process	LogNormal	μ = 4.70	σ = 0.199	–
Heat_Siem	Heat consumption of Siemens process	LogNormal	μ = 5.22	σ = 0.199	–
Elec_CZ	Electricity consumption of Czochralski process	LogNormal	μ = 4.44	σ = 0.199	–
scSi_CZ	Silicon consumption for Czochralski process	LogNormal	μ = 0.07	σ = 0.199	–

[a] MOVPE stands for metal-organic vapor-phase epitaxy, a technique used to grow crystalline semiconductor layers from metal-organic precursors in the vapor phase.
[b] Linking parameter with broad distribution to encompass whole expected range of possibilities.

$$\widetilde{f}(x) = f_0 + \sum_{r=1}^{k} \alpha_r^i \phi_r(x_i) + \sum_{p=1}^{l} \sum_{q=1}^{l'} \beta_{pq}^{ij} \phi_p(x_i)\phi_q(x_j) \quad (3)$$

In this equation, f_0 (zeroth-order term) represents the average value of the original function $f(x)$ across the entire input domain. It captures the baseline behavior of the system, while the remaining terms represent deviations caused by individual variables and their interactions. For practical purposes, the summation is limited to some maximum orders k, l, l'. The error of the model approximation is measured by the scaled distance $\delta(f, \widetilde{f})$, related to the statistical fitness measure R^2 (Eq. (4)).

$$\delta(f, \widetilde{f}) = 1 - R^2 \quad (4)$$

Since the basis functions depend on the probability distribution of the parameters and the coefficients can be calculated by minimizing the square error of the approximation function, the method allows to derive a metamodel simply from input and output data, assuming that the conditions of decomposability and piecewise smoothness are met and that sufficient data points are available. The number of samples needed to generate the metamodel depends on the number of parameters (n) and on the maximum number of coefficients of decomposition (max α and max β) (Eq. (5)).

$$N = 1 + \max\alpha \times n + (\max\beta)^2 \times \frac{n(n-1)}{2} \quad (5)$$

The assumptions behind the HDMR method are consistent with a linear model such as LCA, with the limitation that the method does not support the use of discrete variables that are used in an LCA to represent different technological pathways. Furthermore, the number of samples required is not a limitation. Any number of data points can be generated since the model is a simulation, not reliant on real-world data, with computational power as the only limitation.

Two separate metamodels were developed: one for calculating abiotic depletion and another for climate change impacts. This decision was based on practical considerations. A single metamodel is not required for integration with the ABM, and using separate models avoids the computational burden, however small, of calculating unnecessary outputs during the already demanding ABM simulation. Furthermore, because abiotic depletion and climate change impacts exhibit distinct response behaviors, separating them is expected to improve approximation accuracy.

The design parameters used for each metamodel, summarized in Table 2, were determined through exploratory testing. Specifically, we varied the number of decomposition terms (max α and max β) to identify values that offered a satisfactory trade-off between approximation accuracy and computational cost. Exploratory testing was performed using the climate change model, and the final decomposition settings were then applied to the abiotic depletion model to maintain consistency and reduce redundant testing. Although this approach did not involve formal optimization, the selected parameters resulted in sufficiently accurate approximations for both metamodels, as demonstrated in Section 4.1.

Because the number of required LCA samples depends on the number of decomposition terms, and exploratory testing involves iterating over multiple values, we opted to generate 10,000 simulations. This larger sample size provided flexibility during model tuning and allowed us to assess how many samples were actually needed for stable performance. Additionally, a portion of the dataset was reserved for out-of-sample validation, enabling a robust evaluation of each metamodel's accuracy.

3.4. Case study: Step 3 linking the LCA and ABM

3.4.1. Behavioral foundation

The ABM and metamodel are linked based on an assumption that awareness of the technology's environmental impacts can enhance consumers' positive attitudes towards both circular pathways (e.g.,

Table 2
Metamodel parameters.

Metamodel design parameters	Values
Maximum polynomial order	Optimal values calculated by software
Maximum number of coefficients of decomposition	max α= 10, max β = 4
Number of parameters n	23
Number of samples N	4279

recycling, selling) and adoption pathways (e.g., reuse of second-hand panels) (Fig. 3). This assumption is grounded in Protection Motivation Theory (PMT), a psychological framework that explains how individuals respond to perceived threats. PMT suggests that individuals are motivated to adopt protective behaviors when they evaluate a threat as severe and likely to occur (threat appraisal) and believe their actions can effectively mitigate the threat (coping appraisal) (Rogers, 1975). The connection between the ABM and the metamodel specifically captures how threat appraisal drives changes in attitudes towards adopting more circular strategies. This change in attitude can in turn lead to circular behaviors, consistent with the TPB's premise that attitudes shape behavioral intentions and ultimately behavior itself.

In the ABM, this process is operationalized through a *threshold of concern*, which represents the point at which environmental impacts (e.g., depletion of 0.1 % of total reserves) are perceived as severe enough to trigger a shift in societal attitudes towards more circular practices. Specifically, consumer agents are assumed to be aware of environmental indicators, such as resource depletion or climate change, and when these indicators exceed the threshold, the model simulates an increase in agents' pro-environmental attitudes. This shift assumes the agents' belief that circular behaviors can effectively reduce environmental impacts.

Conversely, when environmental emissions fall below a *threshold of indifference*, the perceived severity of environmental impacts is low, thereby changing the agent's pro-environmental attitudes. That is, if the environmental emissions of solar panels are sufficiently low, agents may no longer view circular behaviors as necessary in addressing resource depletion or climate change. As a result, the motivation to adopt such strategies may decline, as they are no longer perceived as an effective response to the threat.

Evidence from previous studies supports the role of perceived threat and efficacy in motivating pro-environmental behaviors. For instance, Janmaimool (2017) found that people are more likely to engage in recycling and reuse when they perceive pollutants as harmful and likely to affect them. Similarly, Bockarjova and Steg (2014) demonstrated that the perceived severity of the negative impacts of conventional vehicles, along with the perceived effectiveness of electric vehicles to address those impacts, can motivate their adoption.

For simplicity, the thresholds are uniformly applied across all agents, based on the assumption that environmental attitudes can shift collectively in response to shared societal influences. This collective response is driven by perceptions of global or societal markers, such as sustainability targets, eco-labels, or policy initiatives, which serve as common reference points. This reasoning aligns with the work of Albarracin and Shavitt (2018), who emphasize how environmental attitudes are shaped by both individual experiences and broader societal contexts. Their research supports the notion that collective environmental shifts are influenced by widely recognized external cues, reinforcing the validity of applying uniform thresholds in this model. However, a detailed justification for the choice of this threshold extends beyond the illustrative scope of this case study. Thus, the applied thresholds remain

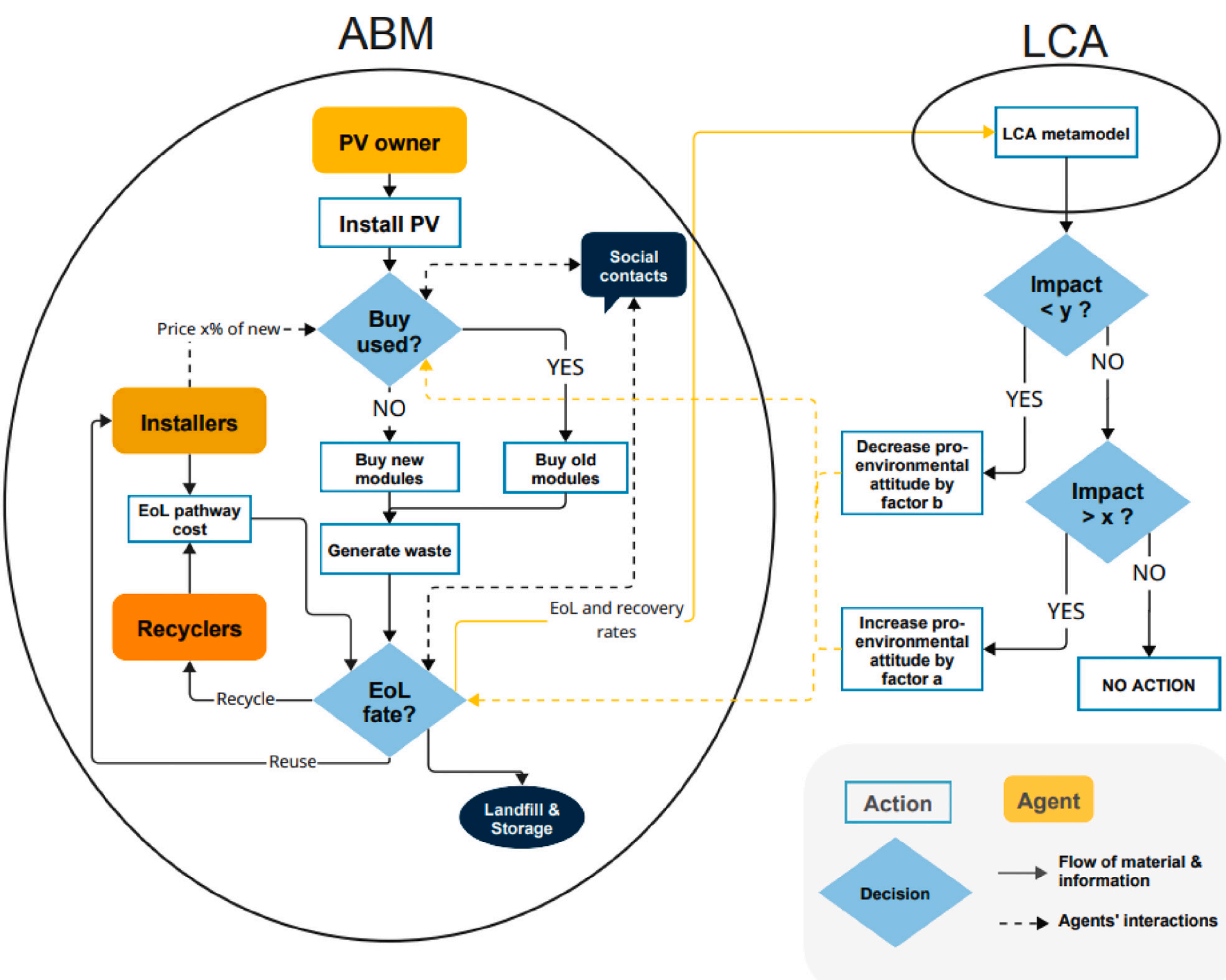

Fig. 3. Schematic representation of the link between the models of Walzberg et al. (2021) and Blanco et al. (2020a) through abiotic depletion and climate change impacts.

hypothetical, serving primarily to demonstrate the model's hard coupling dynamics rather than to establish an empirically validated measure.

3.4.2. Simulation assumptions and scenarios

The hard coupling is implemented in the ABM by monitoring the climate change or abiotic depletion impact category, as calculated by the metamodel, in each tick (or year) of the model. When the impact category exceeds the threshold of concern (e.g., x kg Sb-eq/kWh or x kg CO_2/kWh), it triggers a multiplier effect, where the pro-environmental attitude levels of consumers towards EoL and adoption pathways are increased by a factor (a). In this study, a is set to 2 (representing a 100 % increase). If the impact falls below the threshold, the attitude reverts to its original value.

Different scenarios for this mechanism are explored in Section 4.1.2 by testing progressively lower thresholds of concern. We also compare the hard coupling with the soft coupling, where the calibrated pro-environmental attitudes from Walzberg et al. (2021) are kept fixed. Specifically, we adjust the threshold of concern by starting with the highest impact value observed in the soft coupling and then progressively reduce it in steps of 5 %. This allows us to examine how changes in the threshold affected the model's outcomes, with each reduction representing a different level of environmental severity at which consumer behavior might shift.

When the impacts fall below a threshold of indifference (y kg Sb-eq/kWh or y kgCO_2/kWh), it triggers the decrease of consumers' pro-environmental attitude levels towards circular pathways by a factor (b) within the range of 0 to 1. In this study, b is fixed at 0.5 (representing a 50 % decrease). Section 4.1.3 investigates the influence of this threshold by starting from the minimum impact observed in the threshold-of-concern experiments and increasing it in 5 % increments.

The values of a and b are not empirically derived but were intentionally selected to represent illustrative boundary scenarios of behavioral response. Specifically, $a = 2$ simulates a best-case scenario in which exposure to high environmental impacts sharply increases pro-environmental attitudes. Given that the initial attitude values are drawn from a truncated normal distribution with a mean of 0.544 and a maximum of 1, this doubling will, in most cases, raise the attitude to the upper bound of 1, reflecting an highly optimistic behavioral response. In contrast, $b = 0.5$ represents a worst-case scenario, where declining environmental impacts reduce pro-environmental attitudes by half. These values are used to test the system-level consequences of strong feedback mechanisms, rather than to reproduce real-world behavioral responses. While we do not perform a full sensitivity analysis on a and b, we acknowledge that the assumed strength of feedback has a substantial influence on outcomes. This design choice is aligned with the aim of the case study, which is to demonstrate the analytical flexibility of the integrated ABM–LCA framework.

For each model year (tick), the environmental impacts are calculated using the metamodel based on relevant variables from the ABM. In the initial tick, ABM variables are derived from the baseline scenario for EoL pathways and material recovery rates as outlined by Walzberg et al. (2021). For each subsequent tick the metamodel receives, as input, rates informed by output from the previous model iteration. The Landfill and Reuse fractions, inputs for the metamodel, are calculated from the quantities of recycled, reused, and landfilled panels, which are outputs from the ABM. The recovery rates for most materials, including aluminum, glass, silicon, copper, and silver, are provided according to the baseline scenario from Walzberg et al. (2021), while the recovery rates for gallium and indium (not included in the original ABM) are fixed and remain constant throughout the simulation. The overall integrated model was run 100 times for each analysis.

For clarity, we group reuse and recycling under the term “circular pathways,” distinguishing them from landfilling pathways in the discussion of results.

4. Results and discussion

4.1. Case study integrated model

4.1.1. Metamodel performance

The metamodel is deemed sufficiently accurate for the purpose of integration in the ABM model, with an R-squared of 0.95 for abiotic depletion and 0.82 for climate change (Fig. 4). While the disparity between these values indicates varying levels of precision across impact categories, both are robust enough to reliably capture trends. Moreover, given the inherent uncertainties associated with LCA impacts, the metamodel's approximation provides a solid foundation for the integration.

The sensitivity scores for climate change and abiotic depletion impacts, as illustrated in Fig. 5, indicate that in both cases, the lifetime (LT) of a product and the reuse fraction are influential factors for environmental outcomes. For abiotic depletion, the product lifetime emerges as the most sensitive factor, followed by the reuse fraction, modeled as an extension of product lifetime, and the ratio of landfill to recycling, which ranks as the third most sensitive factor.

For climate change impacts, the sensitivity analysis conducted by Blanco et al. (2025) offers a useful comparison, although their findings partly differ due to the absence of EoL considerations in their model. In both their study and ours, the most sensitive factor is the power consumption during the MOVPE process, which reflects the energy demands of manufacturing processes typical of III-V solar panels. Blanco et al. (2025) identify optimization of the MOVPE process as a top R&D priority. With the introduction of EoL into our model, product lifetime also emerges as a sensitive factor for climate change impacts. Additionally, the reuse fraction, a newly introduced parameter, stands out as another significant contributor.

The high sensitivity of EoL shares is consistent with their intended role in capturing a wide spectrum of potential scenarios, effectively representing the full behavioral space of the ABM (Fig. 5). This sensitivity is to be expected, as the EoL shares are assigned wide distributions to encompass everything that is possible, even if not highly probable. Unlike other parameters constrained by technological limits or natural boundaries, EoL shares are shaped by societal behaviors and decisions, introducing significant variability and flexibility into the model. This sensitivity highlights their value as linking parameters within the integrated model and the importance of using ABM to examine the dynamic and diverse nature of societal choices, which are inherently less predictable and more susceptible to change. Understanding how EoL decisions interact with environmental impacts is essential for gaining system-wide insights and enabling informed decision-making.

For climate change minimization goals, the dominant sensitivity of MOVPE process power consumption suggests that integrating ABM is less critical. Instead, optimizing the MOVPE process itself would be a far more impactful strategy for reducing climate change impacts.

4.1.2. Coupling using threshold of concern

The implementation of a feedback loop between impacts and behavior, by introducing a threshold above which the agent’s pro-environmental attitude increases, results in a large shift towards more circular EoL pathways (Fig. 6). However, we note that the number of simulation runs (100) was selected pragmatically, and the model may not have reached full convergence. As such, the results should be interpreted as demonstrating the framework's functionality rather than providing statistically robust or policy-ready conclusions. Best practices for achieving statistical robustness in ABM studies recommend extensive sensitivity and convergence analyses (Lee et al., 2015; ten Broeke et al., 2021), which we encourage future applications of this framework to adopt.

In the absence of a feedback loop, the model exhibits no variability, consistently defaulting to 100 % landfilling. These results differ from baseline results from Walzberg et al. (2021), which are more optimistic, showing approximately 10 % circular pathways by 2050. This difference

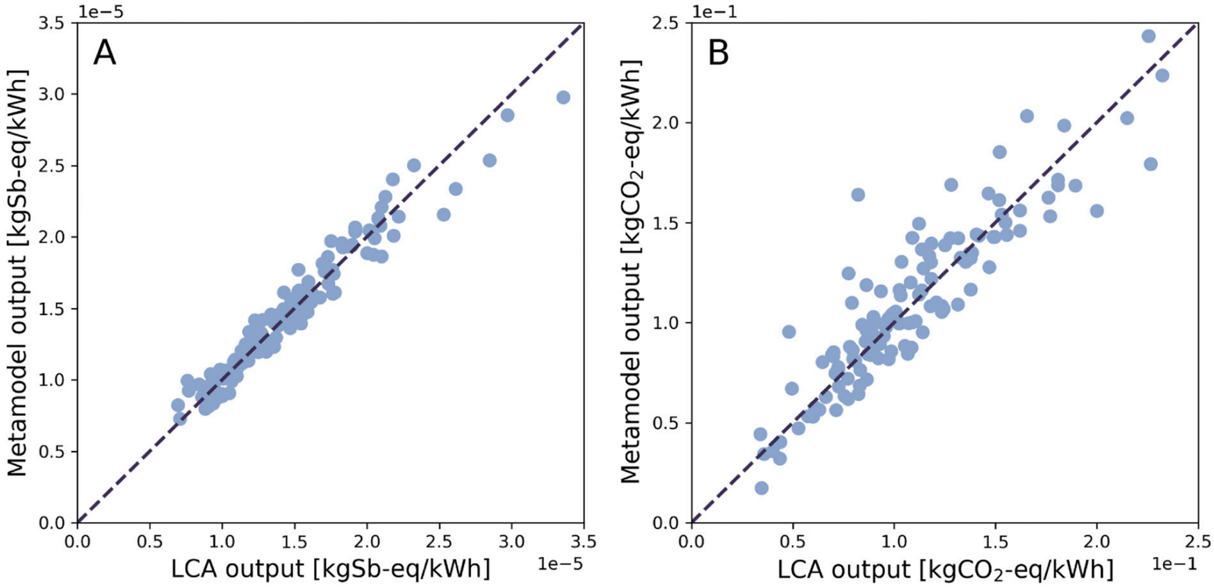

Fig. 4. Plot of the metamodel output compared to LCA output for abiotic resource depletion (A) and climate change (B). R^2 is 0.95 for abiotic depletion and 0.82 for climate change. The dashed line is the 1:1 ratio and each point represents one testing scenario ($n = 128$).

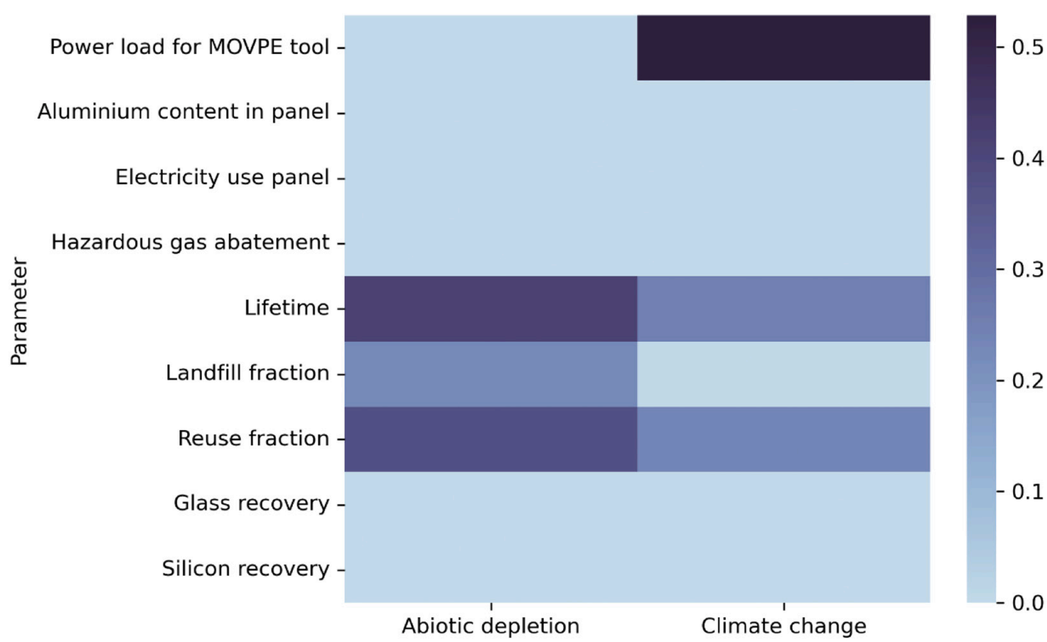

Fig. 5. Total order Sobol sensitivity indices. Only including parameters with sensitivity index >0.001. The recycling fraction is the complement of the landfill fraction.

is expected given the adaptations made to the original model.

Introducing the feedback loop significantly enhances the system's simulated circularity while also amplifying its variability. Stochasticity in the model arises from the network structure and the characteristics of agents, such as their attitudes towards circular EoL pathways and the purchase of second-hand panels. With the feedback loop in place, these attitudes can double, dramatically increasing the effect of initial stochasticity. Moreover, the variability across runs becomes more pronounced over time, as reflected by the shaded area expanding as the model progresses (Figs. 6, 7 and 8). This behavior is explained by the system's path dependency, where outcomes are influenced by the impacts of previous years, creating a “memory” effect in the system. Such path dependency amplifies the divergence of individual runs, leading to an increasingly wider range of outcomes for each consecutive year.

Overall, the results show that lower thresholds generally reduce impacts and increase circular pathways (20 %–100 % for abiotic depletion and 60 %–100 % for climate change) as expected.

As we observed, the variability without a threshold is minimal compared to the variability observed when a threshold is introduced (Fig. 6). However, the distributions also vary across different threshold values (Figs. 7 and 8). For very low thresholds, agents are continually prompted to enhance their pro-environmental behavior in a reinforcing loop because impacts never fall below the concern threshold. With mid-thresholds, agents start in a reinforcing loop, but if impacts drop below the threshold, the system may shift to a balancing loop. This interplay between reinforcing and balancing loops results in increased variability and the emergence of bimodal distributions, reflecting two distinct states, one where impacts are managed effectively and another where

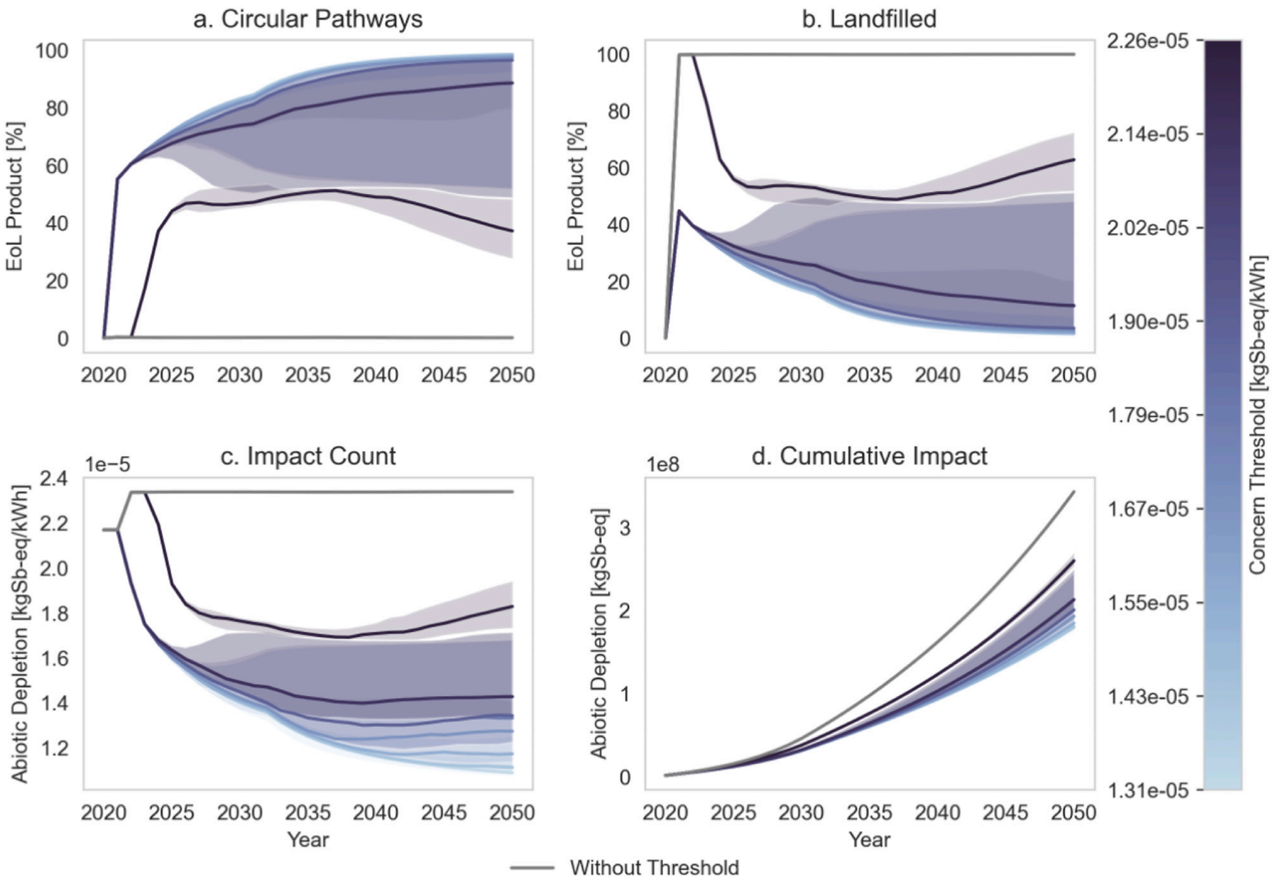

Fig. 6. Effect of introducing a concern threshold for abiotic depletion in the integrated model over time, based on 100 model runs with: (a) Percentage of circular EoL pathways over time under different concern thresholds; (b) Percentage of waste sent to landfill over time under different concern thresholds; (c) Environmental impacts per functional unit over time under different concern thresholds; (d) Cumulative environmental impacts over time under different concern thresholds.[a] The central line represents the median (50th percentile), with the shaded area indicating the range between the 25th and 75th percentiles.
[a]See Figure A2 in the SI for the climate change results.

they rebound. The high variability seen at mid and high thresholds is due to the system's sensitivity to fluctuations. Even minor changes in initial conditions or small perturbations in agent behaviors or network interactions can disproportionately influence the system's overall dynamics. This sensitivity, driven by non-linear interactions and feedback mechanisms, makes outcomes increasingly unpredictable and highlights the system's inherent complexity and non-linearity. This underscores the importance of accounting for variability and non-linear behavior when interpreting these results.

4.1.3. Coupling using threshold of concern and of indifference

The introduction of an indifference threshold, representing a reduction in pro-environmental attitudes under low-impact conditions, extends the original coupling via the concern threshold (Fig. 9). This added mechanism introduces noticeable fluctuations in environmental impact values. To better interpret the source of these apparently chaotic dynamics, single simulation runs can serve as useful illustrations. For example, Fig. A3 in the SI presents a representative run that reveals a characteristic "seesaw" pattern in the trajectory of environmental impact. This oscillation is driven by the behavioral threshold mechanism: when impacts exceed the concern threshold, agents increase pro-environmental actions, which subsequently reduce impacts. Once impacts fall below the indifference threshold, agents reduce their efforts, allowing impacts to rise again. This back-and-forth results in alternating cycles of reinforcement and relaxation, explaining the erratic and jagged appearance of the median trajectories in Fig. 9.

The timing of when the threshold of indifference is crossed appears to be relevant, as it can determine whether the trajectory by year 2050 is on an upward or downward trend. Given the time frame of the observed fluctuations around the concern and indifference thresholds further investigations should extend the simulation time. The introduction of additional thresholds visibly increases the complexity of the system and highlights the challenges we face in properly analyzing and interpreting these dynamics.

While a comprehensive analysis of these dynamics is beyond the scope of this work, it is important to acknowledge that others have highlighted the lack of harmonized and easily applicable analysis approaches (Bodine et al., 2020; Chen et al., 2010; Daly et al., 2022; Medina et al., 2021). Despite advancements in developing increasingly sophisticated ABMs, understanding emergent behavior and its underlying causes in complex sociotechnical systems remains a significant challenge. Typically, conventional statistical and probabilistic methods are used to analyze ABM outputs. Sensitivity analysis is commonly used to identify parameters that strongly affect system behavior (Borgonovo et al., 2022; ten Broeke et al., 2016). To identify tipping points, situations where small changes in parameters trigger regime shifts, more advanced techniques, such as bifurcation diagrams, can be employed. These diagrams map the system's equilibrium points and their stability in relation to varying parameters, offering a deeper understanding of the conditions that trigger regime changes (Ashwin et al., 2012; Bodine et al., 2020). However, manually creating these diagrams in high-dimensional systems is difficult. Machine learning techniques offer a promising approach by simplifying the analysis, reducing dimensionality, and identifying critical thresholds (Fabiani et al., 2024).

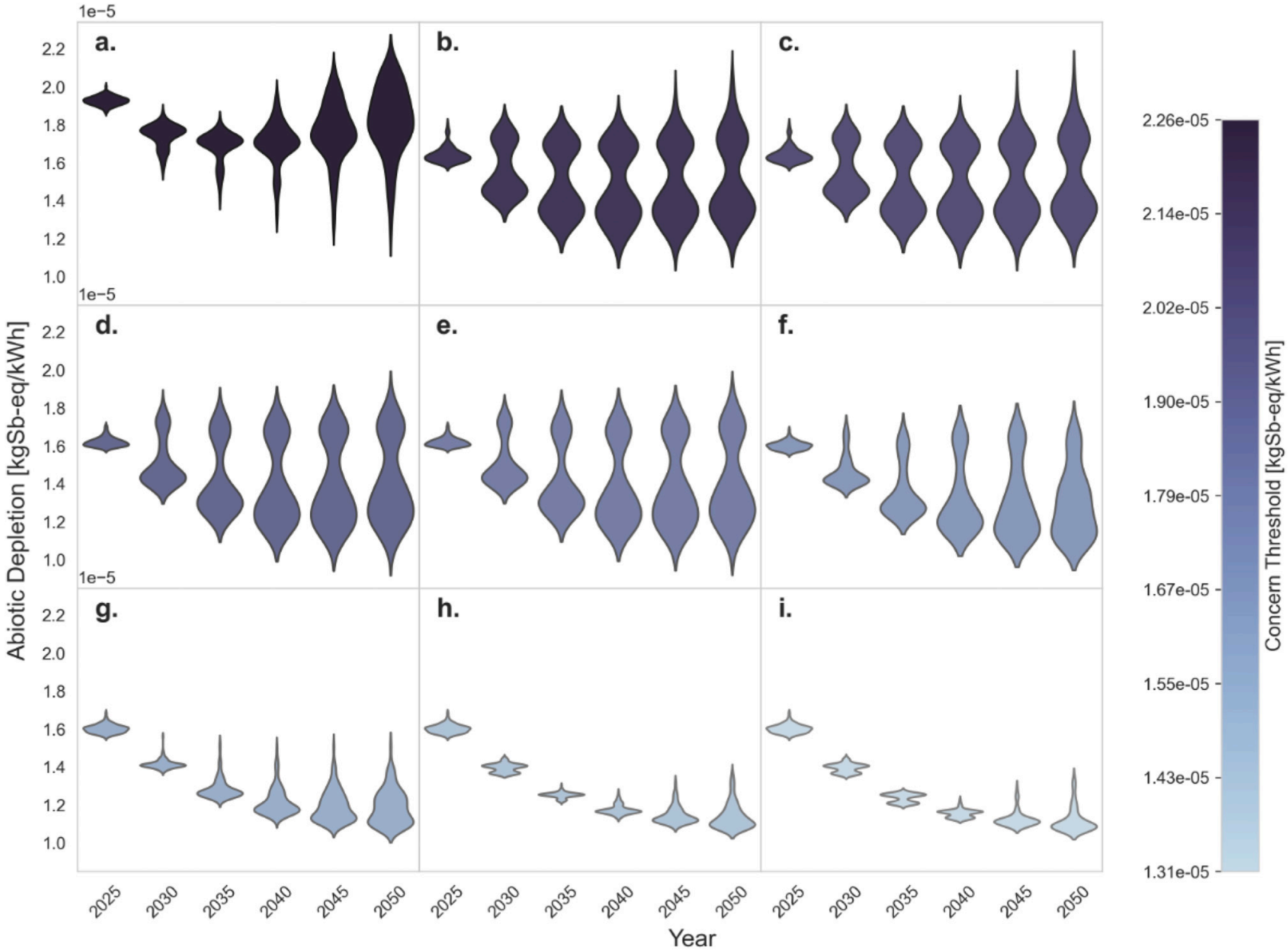

Fig. 7. Violin plot showing distribution of the estimated abiotic depletion for 6 different years of the simulation (100 seeds/runs). Each subplot corresponds to a different threshold of concern: starting from subplot a., with the highest threshold, until subplot i. with the lowest.

4.2. Framework

4.2.1. Temporal dimension

Time plays a critical role in linking LCA and ABM, and the decisions made regarding time in the development of the model should be tailored to each specific application of the framework, as demonstrated in the case study. When implementing a feedback loop between environmental impacts and consumer behavior, it is essential to carefully evaluate the time frame of the environmental impacts to ensure that they align logically with agents' decision-making processes.

In our example application of the framework, the metamodel is derived from a static LCA, but the integration with the ABM introduces a degree of temporal dynamism. Specifically, environmental impacts are recalculated at each time step using behavioral data generated by agents in the previous year. For example, impacts for the year 2049 are calculated based on agents ecisions made in 2048, and these results are then used as feedback to inform decisions in 2050. This creates a sequential feedback loop, where environmental and behavioral dynamics evolve together over time.

However, a key limitation remains: while the foreground behavior in the ABM is dynamic and updated annually, the background LCA data (e.g., supply chain emissions and characterization factors) remains static, and the entire life cycle impact of a product is attributed to a single year. This approach introduces a limitation: the calculated impacts are based on potential emissions rather than temporally distributed, real-time emissions. One way to introduce a more dynamic background is by using temporally explicit LCA, which incorporates time as a variable to reflect changes in background systems. However, to fully synchronize the two models, so that agents make decisions based on impacts reflecting actual emissions, it would be necessary to use modular LCA which divides the life cycle into discrete phases that can be dynamically updated as agents make decisions or external conditions change. In the PV case study, this would allow, for instance, EoL impacts in 2050 to be tied to the actual environmental context of panel manufacturing and electricity use from the panel's installation year in 2020, and attribute use-phase emissions dynamically over the 30-year lifespan.

At this stage, the key question is whether the difference between actual and potential impacts is relevant to the agents' decision-making processes. On one hand, we must consider: What can agents perceive and care about when it comes to environmental impacts? On the other hand, how would agents become aware of these impacts?

The psychological theory reviewed lacks sufficient depth to fully address the first question regarding agent perception (see Section A4 in SI). As for the second question, the information provided to agents in our simulation should not be more precise than the eco-labels or publicly available LCA results they would encounter in real life. Given this, the increase in model accuracy does not justify the increase in computational complexity. However, further improvements may be warranted as more psychological literature on agent perception and behavior becomes available.

Another aspect to consider, although outside of the scope of our demonstrative case study, is that the thresholds for triggering pro-environmental behaviors may need to be treated as time-sensitive, depending on the context and timeframe of the study. For instance, as societal views on sustainability continue to evolve, what constitutes an environmentally responsible decision may change over time, thereby

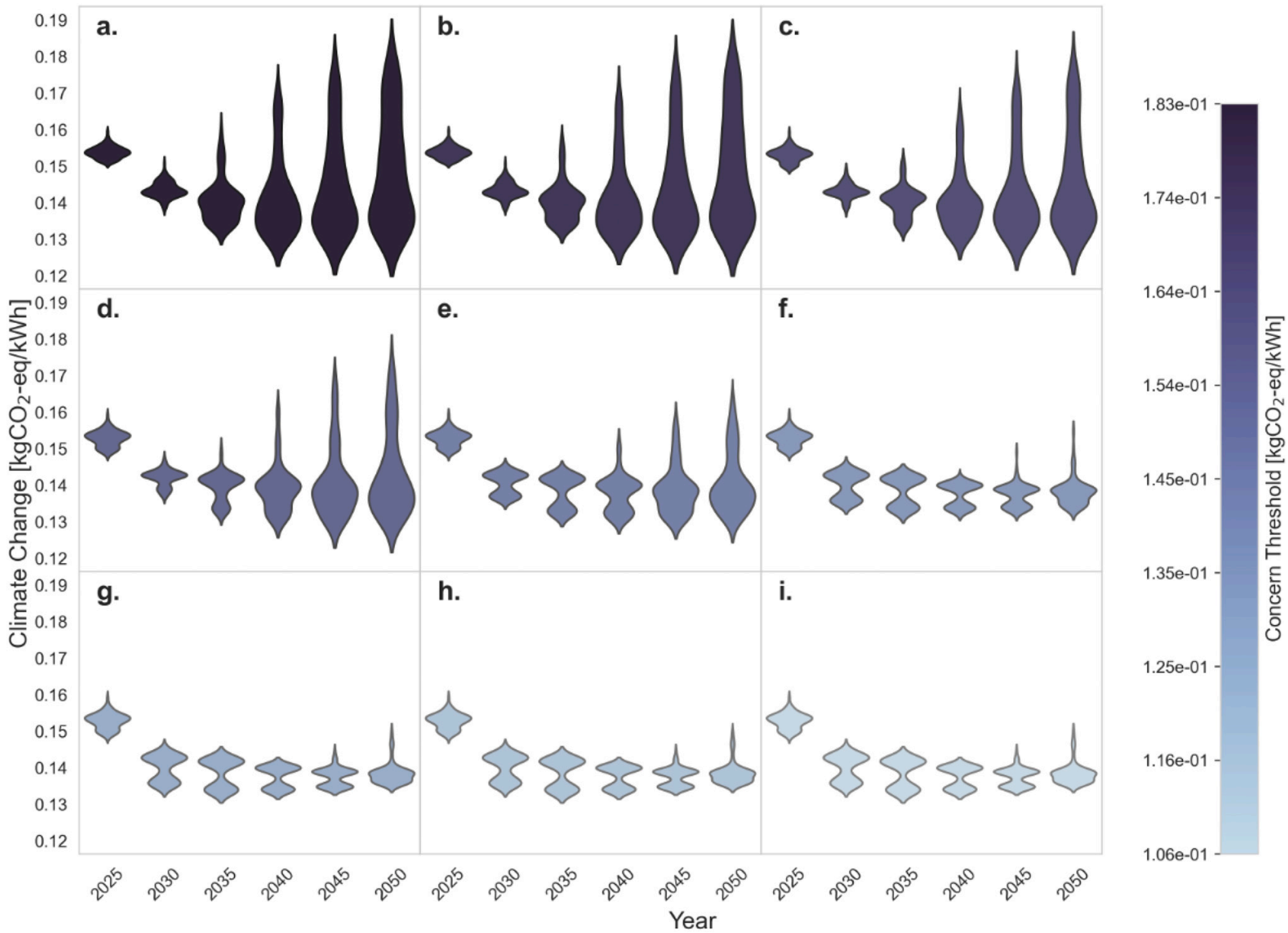

Fig. 8. Violine plot showing distribution of the estimated climate change for 6 different years of the simulation (100 seeds/runs). Each subplot corresponds to a different threshold of concern: starting from subplot a., with the highest threshold, until subplot i. with the lowest.

influencing the critical thresholds that prompt action. This temporal aspect should be accounted for, as shifting perceptions of sustainability can affect both the timing and nature of agents' decisions within the model.

Finally, extending the 30-year time horizon used in the ABM from Walzberg et al. (2021) could provide deeper insights into system dynamics. This is particularly relevant for the PV case study, where the average lifespan of panels is 20 to 30 years. A longer time frame might reveal trends, such as whether the system converges or whether it undergoes recurring cycles or significant shifts in behavior. However, longer simulations also increase uncertainty and variability, as shown in the case study, necessitating careful analysis of long-term dynamics. These insights could be critical for understanding key decision-making factors and their relative contribution to achieving sustainability goals.

4.2.2. Advantages and limitations of using a metamodel

The use of metamodels in the integration of ABM and LCA offers several benefits compared to other approaches. Metamodels, being simple polynomial functions, provide a practical solution by being easily translatable to any programming language and can streamline the computational process reducing the number of parameters involved. One of the primary advantages of metamodels is their low computational intensity, which, while not a major concern for LCA on its own, becomes relevant when considering the broader computational demands of integrated ABM-LCA models. Metamodels simplify the connection between ABM and LCA and eliminate the need to modify LCA matrices or adapt LCA methods. In addition, the use of metamodels enables the creation of open-source models accessible to users without the constraints of proprietary licenses, normally needed for large background Life Cycle Inventory (LCI) databases such as Ecoinvent (Wernet et al., 2016). While the fidelity of a metamodel depends on the training sample size, this is easily addressed in simulation-based studies, where large volumes of LCA output data can be pre-generated to ensure accurate approximation. As demonstrated in our case study, this approach supports efficient coupling between social behavior and environmental feedbacks.

In our case study, the use of the Sobol sensitivity analysis software to generate the RS-HDMR metamodel proved to be a robust and mathematically straightforward approach for integrating LCA with ABM. The metamodel demonstrated high accuracy, with R^2 values of 0.95 for abiotic depletion and 0.82 for climate change, supporting its suitability for efficient and reliable impact prediction. However, one limitation of the software is the support for only a limited set of probability distributions, in particular discrete and pert distributions are excluded. This restriction is notable for LCA, where discrete distributions are often used to model alternative pathways and pert distributions can be used for expert estimates (Blanco et al., 2020b; Mendoza Beltran et al., 2016). On the other hand, the RS-HDMR method has several strengths. RS-HDMR focuses on capturing interactions and effects across multiple dimensions without predefining the function's form, making it ideal for high-dimensional, complex models such as LCA. The main strength of the method relies on its few assumptions: that the function (LCA model in our case) is ANOVA decomposable and that the component functions are piecewise smooth and continuous (Kucherenko, 2013). These assumptions are modest compared to other methods for generating metamodels and are satisfied by most, if not all, LCAs. Furthermore, the RS-

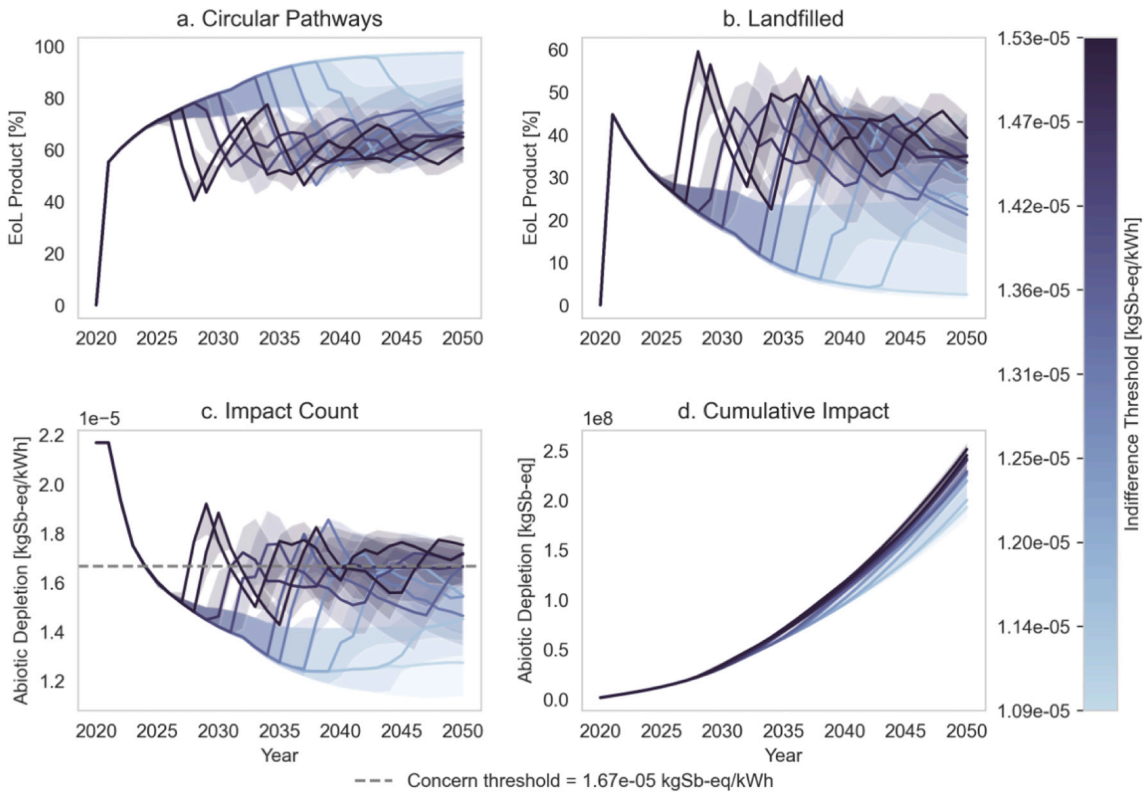

Fig. 9. Effect of adding various indifference thresholds on top of a concern threshold of 1.67e-05kgSb-eq/kWh, over time, based on 100 model runs with: (a) Percentage of circular EoL pathways; (b) Percentage of waste sent to landfill; (c) Environmental impacts per functional unit; (d) Cumulative environmental impact due to abiotic mineral depletion.[a] The central line represents the median (50th percentile), with the shaded area indicating the range between the 25th and 75th percentiles.

[a]See Figure A4–5 in the SI for the corresponding analysis related to climate change

HDMR method leverages the fact that, in most practical problems, only low-order interactions of input variables significantly impact the model output (Rabitz et al., 1999). By concentrating on these interactions and using random sampling to build an efficient approximation, RS-HDMR dramatically reduces the computational time required to build accurate meta-models (Spiessl et al., 2019). Other approaches to derive metamodels, such as simple linear regression and artificial neural networks, offer alternative benefits and can be considered (Fonseca et al., 2003). Simple linear or polynomial regression offers an even more straightforward and interpretable method, however at the cost of operating under strict assumptions of linearity. On the other hand, neural networks can easily capture complex nonlinear relationships, however they necessitate large datasets, significant computational power, and careful hyperparameter tuning (Kleijnen and Sargent, 2000). They are prone to overfitting and often struggle with local minima during training, making them sensitive to initial conditions and optimization methods (Østergård et al., 2018). Other approaches to deriving metamodels may be better suited depending on the specific objectives and contextual needs of each case study.

4.2.3. Applications of the framework in the context of policy making

The dynamic combination of ABM and LCA has the potential to offer unique insights into policy advice in the context of the energy transition. While tight and soft coupling are useful for exploring policy scenarios, a hard-coupled ABM-LCA approach is better at showing how behavior changes over time and revealing unexpected effects.

For instance, the threshold mechanisms implemented in our model could serve as proxies for how behavioral responses might shift under different policies, such as eco-labeling, eco-modulated fees, or awareness campaigns. If future studies provide empirical behavioral data to calibrate these thresholds, such mechanisms could be further refined to policy development and testing. When small increases in environmental impact lead to behavior change, light-touch policies like consumer labels or social norm campaigns may be effective. A real-world example is the European Union's "For Our Planet" campaign, which promotes the principles of reduce, reuse, and repair by emphasizing ecological limits and shared responsibility. Another example of information-based policy, the EU Digital Product Passport (DPP), introduced under the Ecodesign for Sustainable Products Regulation (2024/1781/EU), will require products to disclose environmental performance and end-of-life recommendations, empowering consumer decisions (European Union, 2024). Conversely, if results suggest that only very high impact levels elicit a response, this may support the need for stronger regulatory interventions such as mandatory recycling or extended producer responsibility (EPR) schemes. In the case of solar panels, EPR is mandated across all EU Member States under the Waste Electrical and Electronic Equipment Directive (2012/19/EU), which was later updated to explicitly include PV panels (European Union, 2012; European Commission, 2019).

Despite its analytical strengths, the practical use of ABM in policy advice is often constrained by the complexity involved in presenting and interpreting the model's outcomes. We found that the integration of LCA into ABM introduces additional layers of complexity, making visualization and communication of the results from the case study even more challenging. Unlike conventional models, ABMs produce complex, nonlinear results that are difficult to present in a straightforward manner. This complexity poses a challenge in fields like policy advice, where clear, easily interpretable results are often preferred (Stirling, 2010). Moreover, the absence of a systematic methodology for identifying key variables to monitor and represent them graphically can lead to diverse interpretations of what the model can and should be used for. ABM visualizations need to portray the changes in actions and interactions of agents over time. This is usually addressed using dynamic graphics, often dashboards which provide a more user-friendly interface for interacting with the model, allowing users to adjust parameters (levers) and immediately see the impact on the outcomes (Ruppert et al., 2014). This interactive approach not only enhances understanding by making the relationships between variables more transparent but also allows stakeholders to explore different scenarios in a more intuitive way. For an effective presentation of results from an ABM study an understanding of visual perception and cognition theory is needed (Kornhauser et al., 2009).

4.2.4. Integrated model validation

This study does not include full validation of the integrated ABM-LCA model. Nonetheless, both constituent models are independently grounded in established validation practices. For example, in the case of the ABM from Walzberg et al. (2021), the authors perform multiple types of validation, including theory validation (using empirically validated theories), data validation (calibrating the baseline scenario against empirical data), model output validation (comparing results with projections from authoritative sources like the International Renewable Energy Agency), and face validation (having experts in ABM and PV review the model for expected behavior and meaningful results). The original LCA model by Blanco et al. (2020a) is validated through sensitivity analysis to assess the robustness of its results.

Despite these efforts, both ABM and LCA inherently face challenges with validation. Traditional validation typically involves building a model using historical or experimental data, making predictions, and then testing those predictions against real-world outcomes (Zeigler et al., 2000). This is often not feasible for ABMs due to limited availability of behavioral data and the forward-looking nature of simulated scenarios. Structural validation, which assumes that once a model's internal logic is accurate it remains stable, is particularly problematic in socio-technical systems where behaviors and interactions can shift over time (Heydari and Pennock, 2018). Similarly, LCA models are difficult to validate fully because they estimate potential future impacts rather than direct outcomes. While some foreground data can be validated through measurements or expert review, the validity of results often depends on modeling assumptions and the prevailing scientific consensus around impact assessment methods.

In addition to facing these challenges, future efforts to validate integrated ABM-LCA systems should ideally adopt a holistic strategy, one that includes validation of the individual models as well as the metamodel that governs their integration. Approaches such as "quasi-validation," as proposed by Heydari and Pennock (2018), may offer a viable pathway. These emphasize structural testing, iterative calibration, and examination of system responses under controlled perturbations, helping to assess socio-technical simulations.

4.2.5. Uncertainty and sensitivity analysis

A key limitation of this study is the absence of a comprehensive uncertainty or sensitivity analysis, which is particularly relevant when integrating ABM and LCA. While the framework demonstrates functional coupling, future work should address how uncertainty propagates across both modeling layers. In the context of ABM, global sensitivity analysis has been recognized as essential for understanding how both quantitative inputs and behavioral rules influence emergent outcomes (Borgonovo et al., 2022). However, applying such methods to integrated ABM-LCA systems presents additional challenges, including computational demands and the need to manage multiple sources of uncertainty simultaneously.

Baustert and Benetto (2017) highlight four major sources of uncertainty in integrated modeling, parameter, structural, choice-related, and systemic variability, each of which requires careful treatment to ensure consistent and comparable results. Recent methodological advances show promise in propagating uncertainty from both agent behavior and LCA parameters simultaneously, emphasizing that interactions between different sources of uncertainty can significantly affect results (Baustert et al., 2025). Incorporating such approaches into this framework is a crucial step towards improving transparency, robustness, and eventual policy applicability.

5. Conclusion

The results of the case study demonstrate the viability of the framework and mark a step forward in integrating ABM and LCA for environmental assessments. The use of a metamodel has proven to be an efficient and straightforward method, offering a flexible approach that can be applied to a variety of ABM and LCA studies. By incorporating the dynamics of human behavior and the complexity of energy systems, the framework enables a more comprehensive exploration of uncertainties and emergent phenomena.

While the framework provides valuable insights, interpreting results for policy advice requires further methodological development to effectively address the deep uncertainties inherent in complex systems. Additionally, several aspects of the framework can be extended or refined, including temporal dynamics, validation processes, global sensitivity analysis (GSA), and the visualization and presentation of results. The next step of our research will be to apply the framework to models built from the ground up and to explore ways to ensure the results are accessible and valuable for decision-makers.

This integration has the potential to enrich decision-making processes by accounting for the diversity of perspectives, values, and preferences within a system. By leveraging the strengths of both ABM and LCA, researchers and policymakers can better address critical questions in the energy transition, such as identifying key targets for sustainability and exploring viable paths to achieve them. These advancements enhance our ability to guide and support a more informed transition towards sustainable energy systems.

CRediT authorship contribution statement

Agnese Fuortes: Writing – original draft, Visualization, Software, Methodology. **Carlos Felipe Blanco Rocha:** Writing – review & editing, Methodology, Conceptualization. **Joris T.K. Quik:** Writing – review & editing, Methodology, Conceptualization. **Lynn de Jager:** Writing – original draft. **Willie Peijnenburg:** Writing – review & editing.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the author(s) used ChatGPT in order to improve language and readability. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

This research was funded by the Strategic Program of the Netherlands National Institute for Public Health and the Environment (RIVM), project CHANGE, grant number S/121021/01.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.spc.2025.06.005.

References

Akhshik, M., Bilton, A., Tjong, J., Singh, C.V., Faruk, O., Sain, M., 2022. Prediction of greenhouse gas emissions reductions via machine learning algorithms: toward an artificial intelligence-based life cycle assessment for automotive lightweighting. Sustain. Mater. Technol. 31, e00370. https://doi.org/10.1016/j.susmat.2021.e00370.

Ashwin, P., Wieczorek, S., Vitolo, R., Cox, P., 2012. Tipping points in open systems: bifurcation, noise-induced and rate-dependent examples in the climate system. Philos. Trans. R. Soc. A Math. Phys. Eng. Sci. 370 (1962), 1166–1184. https://doi.org/10.1098/rsta.2011.0306.

Barde, S., van der Hoog, S., 2017. An empirical validation protocol for large-scale agent-based models (SSRN scholarly paper 2992473). Soc. Sci. Res. Netw. https://doi.org/10.2139/ssrn.2992473.

Baustert, P., Benetto, E., 2017. Uncertainty analysis in agent-based modelling and consequential life cycle assessment coupled models: a critical review. J. Clean. Prod. 156, 378–394. https://doi.org/10.1016/j.jclepro.2017.03.193.

Baustert, P., Navarrete Gutiérrez, T.N., Benedetto, E., Rasouli, S., 2025. Propagating uncertainty through coupling of agent-based modelling and life cycle assessment. J. Clean. Prod. 493, 144788. https://doi.org/10.1016/j.jclepro.2025.144788.

Bezdek, R.H., Wendling, R.M., 2002. A half century of long-range energy forecasts: errors made, lessons learned, and implications for forecasting. J. Fusion Energ. 21 (3), 155–172. https://doi.org/10.1023/A:1026208113925.

Bichraoui-Draper, N., Xu, M., Miller, S.A., Guillaume, B., 2015. Agent-based life cycle assessment for switchgrass-based bioenergy systems. Resour. Conserv. Recycl. 103, 171–178. https://doi.org/10.1016/j.resconrec.2015.08.003.

Blanco, C.F., Cucurachi, S., Dimroth, F., Guinée, J.B., Peijnenburg, W.J.G.M., Vijver, M. G., 2020a. Environmental impacts of III–V/silicon photovoltaics: life cycle assessment and guidance for sustainable manufacturing. Energ. Environ. Sci. 13 (11), 4280–4290. https://doi.org/10.1039/D0EE01039A.

Blanco, C.F., Cucurachi, S., Guinée, J.B., Vijver, M.G., Peijnenburg, W.J.G.M., Trattnig, R., Heijungs, R., 2020b. Assessing the sustainability of emerging technologies: a probabilistic LCA method applied to advanced photovoltaics. J. Clean. Prod. 259, 120968. https://doi.org/10.1016/j.jclepro.2020.120968.

Blanco, C.F., Behrens, P., Vijver, M., Peijnenburg, W., Quik, J., Cucurachi, S., 2025. A framework for guiding safe and sustainable-by-design innovation. J. Ind. Ecol. 29 (1), 47–65. https://doi.org/10.1111/jiec.13609.

Bockarjova, M., Steg, L., 2014. Can protection motivation theory predict pro-environmental behavior? Explaining the adoption of electric vehicles in the Netherlands. Glob. Environ. Chang. 28, 276–288. https://doi.org/10.1016/j.gloenvcha.2014.06.010.

Bodine, E.N., Panoff, R.M., Voit, E.O., Weisstein, A.E., 2020. Agent-based modeling and simulation in mathematics and biology education. Bull. Math. Biol. 82 (8), 101. https://doi.org/10.1007/s11538-020-00778-z.

Borgonovo, E., Pangallo, M., Rivkin, J., Rizzo, L., Siggelkow, N., 2022. Sensitivity analysis of agent-based models: a new protocol. Computational and Mathematical Organization Theory 28 (1), 52–94. https://doi.org/10.1007/s10588-021-09358-5.

ten Broeke, G., van Voorn, G., Ligtenberg, A., 2016. Which sensitivity analysis method should I use for my agent-based model? J. Artif. Soc. Soc. Simul. 19 (1), 5. https://doi.org/10.18564/jasss.2857.

ten Broeke, G., van Voorn, G., Ligtenberg, A., Molenaar, J., 2021. The use of surrogate models to analyse agent-based models. J. Artif. Soc. Soc. Simul. 24 (2), 3. https://doi.org/10.18564/jasss.4530.

Carrington, G., Stephenson, J., 2018. The politics of energy scenarios: are international energy agency and other conservative projections hampering the renewable energy transition? Energy Res. Soc. Sci. 46, 103–113. https://doi.org/10.1016/j.erss.2018.07.011.

Chen, C.-C., Clack, C.D., Nagl, S.B., 2010. Identifying multi-level emergent behaviors in agent-directed simulations using complex event type specifications. Simulation 86 (1), 41–51. https://doi.org/10.1177/0037549709106692.

Dabbaghi, F., Tanhadoust, A., Nehdi, M.L., Nasrollahpour, S., Dehestani, M., Yousefpour, H., 2021. Life cycle assessment multi-objective optimization and deep belief network model for sustainable lightweight aggregate concrete. J. Clean. Prod. 318, 128554. https://doi.org/10.1016/j.jclepro.2021.128554.

Daly, A.J., De Visscher, L., Baetens, J.M., De Baets, B., 2022. Quo vadis, agent-based modelling tools? Environ. Model. Softw. 157, 105514. https://doi.org/10.1016/j.envsoft.2022.105514.

Dam, K.H., Nikolic, I., Lukszo, Z. (Eds.), 2013. Agent-based modelling of socio-technical systems. Springer Netherlands. https://doi.org/10.1007/978-94-007-4933-7.

Davis, C., Nikolić, I., Dijkema, G.P.J., 2009. Integration of life cycle assessment into agent-based modeling. J. Ind. Ecol. 13 (2), 306–325. https://doi.org/10.1111/j.1530-9290.2009.00122.x.

European Commission, 2019. Commission delegated directive (EU) 2019/184 of 5 November 2018 amending annex III to directive 2012/19/EU on waste electrical and electronic equipment (WEEE). Official Journal of the European Union L 39, 128–130. https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32019L0184.

European Union, 2012. Directive 2012/19/EU of the European Parliament and of the Council of 4 July 2012 on Waste Electrical and Electronic Equipment (WEEE). Official Journal of the European Union L 197, 38–71. https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A32012L0019.

European Union, 2024. Regulation (EU) 2024/1781 of the European Parliament and of the Council of 13 March 2024 on the Ecodesign for Sustainable Products. Official Journal of the European Union L 202, 1–48. https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A32024R1781.

Fabiani, G., Evangelou, N., Cui, T., Bello-Rivas, J.M., Martin-Linares, C.P., Siettos, C., Kevrekidis, I.G., 2024. Task-oriented machine learning surrogates for tipping points of agent-based models. Nat. Commun. 15 (1), 4117. https://doi.org/10.1038/s41467-024-48024-7.

Fonseca, D.J., Navaresse, D.O., Moynihan, G.P., 2003. Simulation metamodeling through artificial neural networks. Eng. Appl. Artif. Intel. 16 (3), 177–183. https://doi.org/10.1016/S0952-1976(03)00043-5.

Fuortes, A., Quik, J., Blanco Rocha, C.F., 2025. PV-ABM-LCA (Version 1.0) [Computer software]. National Institute for Public Health and the Environment. https://doi.org/10.21945/28ef999c-a59f-4217-9a1f-49f285b401af.

Geels, F.W., Sovacool, B.K., Schwanen, T., Sorrell, S., 2017. Sociotechnical transitions for deep decarbonization. Science 357 (6357), 1242–1244. https://doi.org/10.1126/science.aao3760.

Hansen, P., Liu, X., Morrison, G.M., 2019. Agent-based modelling and socio-technical energy transitions: a systematic literature review. Energy Res. Soc. Sci. 49, 41–52. https://doi.org/10.1016/j.erss.2018.10.021.

Heydari, B., Pennock, M.J., 2018. Guiding the behavior of sociotechnical systems: the role of agent-based modeling. Syst. Eng. 21 (3), 210–226. https://doi.org/10.1002/sys.21435.

Hicks, A., 2022. Seeing the people in LCA: agent based models as one possibility. Resources, Conservation & Recycling Advances 15, 200091. https://doi.org/10.1016/j.rcradv.2022.200091.

ISO, 2016. Environmental management—Life cycle assessment—Principles and framework. (ISO 14040:2006). https://www.iso.org/standard/37456.html.

Janmaimool, P., 2017. Application of protection motivation theory to investigate sustainable waste management behaviors. Sustainability 9 (7). https://doi.org/10.3390/su9071079.

Jian, S.-M., Wu, B., Hu, N., 2021. Environmental impacts of three waste concrete recycling strategies for prefabricated components through comparative life cycle assessment. J. Clean. Prod. 328, 129463. https://doi.org/10.1016/j.jclepro.2021.129463.

Karamian, F., Mirakzadeh, A.A., Azari, A., 2023. Application of multi-objective genetic algorithm for optimal combination of resources to achieve sustainable agriculture based on the water-energy-food nexus framework. Sci. Total Environ. 860, 160419. https://doi.org/10.1016/j.scitotenv.2022.160419.

Khang, D.S., Tan, R.R., Uy, O.M., Promentilla, M.A.B., Tuan, P.D., Abe, N., Razon, L.F., 2017. Design of experiments for global sensitivity analysis in life cycle assessment: the case of biodiesel in Vietnam. Resources, Conservation and Recycling 119, 12–23. https://doi.org/10.1016/j.resconrec.2016.08.016.

Kleijnen, J.P.C., Sargent, R.G., 2000. A methodology for fitting and validating metamodels in simulation. Eur. J. Oper. Res. 120 (1), 14–29. https://doi.org/10.1016/S0377-2217(98)00392-0.

Kornhauser, D., Wilensky, U., Rand, W., 2009. Design guidelines for agent based model visualization. J. Artif. Soc. Soc. Simul. 12.

Kucherenko, S., 2013. SOBOLHDMR: A general-purpose modeling software. In: Polizzi, K.M., Kontoravdi, C. (Eds.), Synthetic Biology. Humana Press, pp. 191–224. https://doi.org/10.1007/978-1-62703-625-2_16.

Lamperti, F., Roventini, A., Sani, A., 2018. Agent-based model calibration using machine learning surrogates. J. Econ. Dyn. Control. 90, 366–389. https://doi.org/10.1016/j.jedc.2018.03.011.

Lan, L., Wood, K.L., Yuen, C., 2019. A holistic design approach for residential net-zero energy buildings: a case study in Singapore. Sustain. Cities Soc. 50. https://doi.org/10.1016/j.scs.2019.101672.

Lee, J.-S., Filatova, T., Ligmann-Zielinska, A., Mahmooei, B.H., Stonedahl, F., Lorscheid, I., Voinov, A., Polhill, J.G., Sun, Z., Parker, D.C., 2015. The complexities of agent-based modeling output analysis. J. Artif. Soc. Soc. Simul. 18 (4), 1–27. https://doi.org/10.18564/jasss.2897.

Li, G., Wang, S.-W., Rabitz, H., 2002. Practical approaches to construct RS-HDMR component functions. Chem. A Eur. J. 106 (37), 8721–8733. https://doi.org/10.1021/jp014567t.

Li, G., Hu, J., Wang, S.-W., Georgopoulos, P.G., Schoendorf, J., Rabitz, H., 2006. Random sampling-high dimensional model representation (RS-HDMR) and orthogonality of its different order component functions. Chem. A Eur. J. 110 (7), 2474–2485. https://doi.org/10.1021/jp054148m.

Li, Y.F., Ng, S.H., Xie, M., Goh, T.N., 2010. A systematic comparison of metamodeling techniques for simulation optimization in decision support systems. Appl. Soft Comput. 10 (4), 1257–1273. https://doi.org/10.1016/j.asoc.2009.11.034.

Li, P., Chen, B., Cui, Q., 2023. A probabilistic life-cycle assessment of carbon emission from magnesium phosphate cementitious material with uncertainty analysis. J. Clean. Prod. 427, 139164. https://doi.org/10.1016/j.jclepro.2023.139164.

Ligmann-Zielinska, A., Siebers, P.-O., Magliocca, N., Parker, D.C., Grimm, V., Du, J., Cenek, M., Radchuk, V., Arbab, N.N., Li, S., Berger, U., Paudel, R., Robinson, D.T., Jankowski, P., An, L., Ye, X., 2020. 'One size does not fit all': a roadmap of purpose-driven mixed-method pathways for sensitivity analysis of agent-based models. J. Artif. Soc. Soc. Simul. 23 (1), 6. https://doi.org/10.18564/jasss.4201.

MacLeod, M., Nagatsu, M., 2018. What does interdisciplinarity look like in practice: mapping interdisciplinarity and its limits in the environmental sciences. Studies in History and Philosophy of Science Part A 67, 74–84. https://doi.org/10.1016/j.shpsa.2018.01.001.

Marvuglia, A., Gutiérrez, T.N., Baustert, P., Benetto, E., Marvuglia, A., Gutiérrez, T.N., Baustert, P., Benetto, E., 2018. Implementation of agent-based models to support life cycle assessment: a review focusing on agriculture and land use. AIMS Agric. Food 3 (4), 535. https://doi.org/10.3934/agrfood.2018.4.535.

Marvuglia, A., Bayram, A., Baustert, P., Gutiérrez, T.N., Igos, E., 2022. Agent-based modelling to simulate farmers' sustainable decisions: farmers' interaction and

resulting green consciousness evolution. J. Clean. Prod. 332, 129847. https://doi.org/10.1016/j.jclepro.2021.129847.
Medina, M., Huffaker, R., Muñoz-Carpena, R., Kiker, G., 2021. An empirical nonlinear dynamics approach to analyzing emergent behavior of agent-based models. AIP Adv. 11 (3), 035133. https://doi.org/10.1063/5.0023116.
Mendoza Beltran, A., Heijungs, R., Guinée, J., Tukker, A., 2016. A pseudo-statistical approach to treat choice uncertainty: the example of partitioning allocation methods. Int. J. Life Cycle Assess. 21 (2), 252–264. https://doi.org/10.1007/s11367-015-0994-4.
Micolier, A., Loubet, P., Taillandier, F., Sonnemann, G., 2019. To what extent can agent-based modelling enhance a life cycle assessment? Answers based on a literature review. J. Clean. Prod. 239, 118123. https://doi.org/10.1016/j.jclepro.2019.118123.
Miller, S.A., Moysey, S., Sharp, B., Alfaro, J., 2013. A stochastic approach to model dynamic systems in life cycle assessment. J. Ind. Ecol. 17 (3), 352–362. https://doi.org/10.1111/j.1530-9290.2012.00531.x.
Morgan, M.G., Keith, D.W., 2008. Improving the way we think about projecting future energy use and emissions of carbon dioxide. Clim. Change 90 (3), 189–215. https://doi.org/10.1007/s10584-008-9458-1.
Mutel, C., 2017. Brightway: An open source framework for life cycle assessment. J. Open Source Softw. 2 (12), 236. https://doi.org/10.21105/joss.00236.
Navarrete Gutiérrez, T.N., Rege, S., Marvuglia, A., Benetto, E., 2015. Introducing LCA results to ABM for assessing the influence of sustainable behaviours. In: Bajo, J., Hernández, J.Z., Mathieu, P., Campbell, A., Fernández-Caballero, A., Moreno, M.N., Julián, V., Alonso-Betanzos, A., Jiménez-López, M.D., Botti, V. (Eds.), Trends in Practical Applications of Agents, Multi-Agent Systems and Sustainability. Springer International Publishing, pp. 185–196. https://doi.org/10.1007/978-3-319-19629-9_21.
Onat, N.C., Noori, M., Kucukvar, M., Zhao, Y., Tatari, O., Chester, M., 2017. Exploring the suitability of electric vehicles in the United States. Energy 121, 631–642. https://doi.org/10.1016/j.energy.2017.01.035.
Østergård, T., Jensen, R.L., Maagaard, S.E., 2018. A comparison of six metamodeling techniques applied to building performance simulations. Appl. Energy 211, 89–103. https://doi.org/10.1016/j.apenergy.2017.10.102.
Papadopoulos, S., Azar, E., 2016. Integrating building performance simulation in agent-based modeling using regression surrogate models: a novel human-in-the-loop energy modeling approach. Energ. Buildings 128, 214–223. https://doi.org/10.1016/j.enbuild.2016.06.079.
Parry, H.R., Topping, C.J., Kennedy, M.C., Boatman, N.D., Murray, A.W.A., 2013. A Bayesian sensitivity analysis applied to an agent-based model of bird population response to landscape change. Environ. Model. Software 45, 104–115. https://doi.org/10.1016/j.envsoft.2012.08.006.
Polo-Mendoza, R., Martinez-Arguelles, G., Peñabaena-Niebles, R., 2023. Environmental optimization of warm mix asphalt (WMA) design with recycled concrete aggregates (RCA) inclusion through artificial intelligence (AI) techniques. Results in Engineering 17, 100984. https://doi.org/10.1016/j.rineng.2023.100984.
Rabitz, H., Aliş, Ö.F., Shorter, J., Shim, K., 1999. Efficient input—Output model representations. Comput. Phys. Commun. 117 (1), 11–20. https://doi.org/10.1016/S0010-4655(98)00152-0.
Rivera, J.L., Sutherland, J.W., 2015. A design of experiments (DOE) approach to data uncertainty in LCA: application to nanotechnology evaluation. Clean Techn. Environ. Policy 17 (6), 1585–1595. https://doi.org/10.1007/s10098-014-0890-9.
Rogers, R.W., 1975. A protection motivation theory of fear appeals and attitude change. J. Psychol. 91 (1), 93–114. https://doi.org/10.1080/00223980.1975.9915803.
Ruppert, T., Bernard, J., Ulmer, A., Lücke-Tieke, H., Kohlhammer, J., 2014. Visual access to an agent-based simulation model to support political decision making. In: Proceedings of the 14th International Conference on Knowledge Technologies and Data-Driven Business, pp. 1–8. https://doi.org/10.1145/2637748.2638410.
Scoones, I., Stirling, A., 2020. Uncertainty and the politics of transformation. In: The Politics of Uncertainty. Routledge.
Shekoohiyan, S., Hadadian, M., Heidari, M., Hosseinzadeh-Bandbafha, H., 2023. Life cycle assessment of Tehran municipal solid waste during the COVID-19 pandemic and environmental impacts prediction using machine learning. Case Studies in Chemical and Environmental Engineering 7, 100331. https://doi.org/10.1016/j.cscee.2023.100331.
Spiessl, S.M., Kucherenko, S., Becker, D.-A., Zaccheus, O., 2019. Higher-order sensitivity analysis of a final repository model with discontinuous behaviour using the RS-HDMR meta-modeling approach. Reliability Engineering & System Safety 187, 149–158. https://doi.org/10.1016/j.ress.2018.12.004.
Steubing, B., de Koning, D., Haas, A., Mutel, C.L., 2020. The activity browser—An open source LCA software building on top of the brightway framework. Software Impacts 3, 100012. https://doi.org/10.1016/j.simpa.2019.100012.
Stirling, A., 2010. Keep it complex. Nature 468 (7327), 1029–1031. https://doi.org/10.1038/4681029a.
van Strien, M., Huber, S., Anderies, J., Grêt-Regamey, A., 2019. Resilience in social-ecological systems: identifying stable and unstable equilibria with agent-based models. Ecol. Soc. 24 (2). https://doi.org/10.5751/ES-10899-240208.
Thiele, J.C., Kurth, W., Grimm, V., 2014. Facilitating parameter estimation and sensitivity analysis of agent-based models: a cookbook using NetLogo and R. J. Artif. Soc. Soc. Simul. 17 (3). https://doi.org/10.18564/jasss.2503.
Walzberg, J., Dandres, T., Merveille, N., Cheriet, M., Samson, R., 2019. Assessing behavioural change with agent-based life cycle assessment: application to smart homes. Renew. Sustain. Energy Rev. 111, 365–376. https://doi.org/10.1016/j.rser.2019.05.038.
Walzberg, J., Carpenter, A., Heath, G.A., 2021. Role of the social factors in success of solar photovoltaic reuse and recycle programmes. Nat. Energy 6 (9), 913–924. https://doi.org/10.1038/s41560-021-00888-5.
Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., Weidema, B., 2016. The ecoinvent database version 3 (part I): overview and methodology. Int. J. Life Cycle Assess. 21 (9), 1218–1230. https://doi.org/10.1007/s11367-016-1087-8.
Zeigler, B.P., Praehofer, H., Kim, T.G, 2000. Theory of Modeling and Simulation. Academic Press.
Zuniga, M.M., Kucherenko, S., Shah, N., 2013. Metamodelling with independent and dependent inputs. Comput. Phys. Commun. 184 (6), 1570–1580. https://doi.org/10.1016/j.cpc.2013.02.005.
Zupko, R., 2021. Application of agent-based modeling and life cycle sustainability assessment to evaluate biorefinery placement. Biomass Bioenergy 144, 105916. https://doi.org/10.1016/j.biombioe.2020.105916.