

Integrating sociotechnical factors to assess efficacy of PV recycling and reuse interventions

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Abstract

By 2050, the cumulative mass of end-of-life photovoltaic (PV) modules may reach 80 million metric tons globally. The impacts could be mitigated by circular economy (CE) strategies including module recycling, repair, and reuse. However, previous studies of PV circularity omit consideration of critical social factors. We use a novel agent-based model to integrate social aspects with techno-economic factors—providing a more realistic assessment of circularity potential for previously studied CE interventions and assessing additional interventions that cannot be analyzed using techno-economic analysis alone. We also performed a global sensitivity analysis using a machine-learning metamodel. We show that excluding social factors underestimates the effect of lower recycling prices on PV material circularity. Interventions aimed at changing customer attitudes about used PV boost module reuse, although used modules can only satisfy a third of US demand during 2020–2050, suggesting that reuse should be complemented by recycling.

Keywords: Circular economy; agent-based modeling; socio-technical systems; circular strategies; machine learning; photovoltaics.

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1. (Introduction)

Soaring global deployment of solar photovoltaics (PV) could mitigate problems related to energy generation but may exacerbate other issues. PV manufacturing depletes scarce resources such as silver, tellurium, and copper^{1,2}. For instance, silver production could peak by 2030, with a risk of demand outstripping supply around 2075³. Although minerals and metals are essential for the transition to a low-carbon society, increased use could aggravate social and ecological problems⁴. Large-scale PV deployment also will produce substantial amounts of end-of-life (EOL) PV materials. By 2050, a cumulative 80 million metric tons of PV modules are expected to reach EOL globally, with 10 million metric tons in the United States (US) alone⁵.

Outcomes associated with increased PV deployment depend on the economic approach applied. In today's predominantly linear economy, resources are extracted to manufacture goods, which are later discarded. The alternative circular economy (CE) model could mitigate resource and ecological challenges⁶ by encouraging dematerialization and the recovery and reuse of products and materials^{6,7}. Challenges to a PV CE include low recycling rates^{3,8}, non-specialized PV recycling⁹ resulting in low material recovery rates and profits⁸, difficult separation of module components³, and product reuse limited by consumer awareness and attitude toward used products as well as current policy¹⁰.

Adopting a social viewpoint to complement other perspectives could increase the effectiveness of circularity-promoting interventions. Social behaviors could play a critical role in developing secondary PV markets and managing EOL PV, because psychological and behavioral traits often undermine the viability of technical solutions¹¹⁻¹⁴. Sovacool and Griffiths, for instance, report that culturally rooted driving behaviors influence adoption of fuel-efficient vehicles and ridesharing services¹⁴. However, current studies of material circularity are limited to technical and economic material efficiency potentials and do not account for consumer behavior^{13,15}. This assessment means that major changes in the way CE is analyzed need to be undertaken^{12,16,17}.

We help fill this gap by incorporating social considerations into an exploration of the techno-economic, market, and policy conditions that may maximize material circularity of the dominant crystalline-silicon (c-Si) PV module technology. We apply a novel agent-based model (ABM) to represent multiple actors involved with the PV life cycle as well as social factors (attitude and peer influence) constraining CE strategies and build a machine-learning (ML) metamodel to conduct a global sensitivity analysis. An ABM is well suited for studying the CE transition because it considers temporal aspects, adopts a systemic view, and accounts for human decisions and interactions between actors¹⁶, exploiting recent advances in behavioral economics and psychology^{16,18-20}. ABMs have been used to study CE scenarios in relation to waste management²¹⁻²⁴, but no previous model has included secondary market dynamics

underlying the reuse CE strategy. Many ABM studies have addressed PV adoption¹⁹, but the method has never been used to investigate renewable technologies through EOL.

By integrating social considerations, we not only analyze the factors affecting PV CE scenarios more comprehensively than previous studies have, but we also explore types of CE interventions—such as strengthening warranties for used PV modules and “seeding” used modules to encourage secondary-market development—that cannot be assessed using techno-economic analysis alone. The result is a fuller picture of the options available for promoting PV circularity and a fuller picture of the potential effectiveness of those options separately and in combination.

2. Results and discussion

In our ABM, four types of agents (PV owners, installers, recyclers, and manufacturers) and five EOL management options (repair, reuse, recycling, landfilling, and storage) are defined (Supplementary Figure 1), focusing on CE strategies that have been proposed by stakeholders as likely to contribute most to the CE in the future²⁵. Landfilling and storage are included because those options have been reported in the US^{26,27}. Two purchasing options are also modeled: the purchase of new or used PV modules. For each type of agent, behavioral rules are defined based on the theory of planned behavior (TPB), which is one of the most influential theories used to explain human behavior¹³ and accounts for various factors affecting human decisions, such as economics and peer influence (Supplementary Table 1).

Our ABM simulates current US conditions, although changing several rules and other parameters would enable it to simulate EOL decisions for PV modules anywhere in the world. The European Union, where PV modules must be recycled at EOL based on waste electrical and electronic equipment (WEEE) regulations, is the most constrained region because only few pathways are allowed. The US is projected to have the second-largest amount of EOL modules by 2050⁵, and landfilling is considerably cheaper than recycling²⁶. In this challenging environment for a PV CE, it is vital to identify the most effective and cost-efficient strategies or combinations of strategies to achieve maximum material circularity. To do so, we assess not only the fraction of EOL mass that avoids being landfilled (and stored), but also societal costs (i.e., net costs of manufacturers, recyclers, and installers) and recyclers and installers net revenue, because those metrics are relevant to assuring the sustainability of the CE. Dynamic factors considered include the PV module failure rate and the learning effect for module recycling—that is, the decrease in recycling costs with increasing recycled volumes due to factors such as economies of scale and technological advancement²⁸. Our ABM is also stochastic to account for variability in some parameters, such as landfill costs, and to enable advanced sensitivity and uncertainty analysis (Supplementary Table 1). We run 30 simulations for each scenario from 2020 to 2050 and present means in the paper’s main body; we selected

the number of simulations based on a stability analysis reported in Supplementary Figure 2. The ABM differs from similar waste-management models by including decisions related to the demand and supply sides of reuse, accounting for technical factors such as the recycling learning effect, and extending reported metrics²¹⁻²⁴. Our approach also differs from current literature on PV EOL management in that behavioral aspects are captured to better characterize the CE transition. We start by providing an overview of CE scenarios, showing that many interventions besides regulations could promote circularity (Figure 1, Supplementary Table 2, Supplementary Figures 3 and 4). In the subsequent subsection, we further explore several of the interventions from Figure 1.

The baseline scenario reflects current US conditions, calibrated to available evidence, and reproduces today's low recycling and reuse rates^{8,29} as well as projected cumulative PV capacity and EOL modules based on the literature⁵. In this scenario, 500 GW of PV will be installed in the US between 2020 and 2050, generating 9.1 million metric tons of PV waste during the same period (Supplementary Figure 5), average initial recycling costs are \$28/module, and average landfill costs are \$1.38/module. Most modules are landfilled (83% by mass), while 1.2% are reused and 9.5% are recycled. Only 80% of a given module's materials is recovered through recycling in the baseline scenario, because the assumed recycling process entails simple mechanical separation recovering only the aluminum frame and glass sheets from EOL modules⁹. Thus, the material recycling rate is 7.7%, equivalent to 0.7 million metric tons cumulatively through 2050 (Figure 1, scenario i). We express all EOL rates in mass percentage of materials, including manufacturing waste, and represent cumulative amounts in 2050 unless otherwise specified. In this baseline scenario, recycling is not profitable in any year, even when accounting for the learning effect and revenue from recovered materials, so PV owners must pay a recycling fee (Supplementary Figure 5).

Techno-economic interventions could improve PV materials circularity. Research and development in recycling technologies could yield lower costs (Figure 1, scenario c), better performance, or both (Figure 1, scenarios b and f). Research and development to improve module durability would lower the amount of PV EOL materials generated (Figure 1, scenario e). Market interventions such as better warranties for recovered modules (Figure 1, scenario g), higher landfill costs (Figure 1, scenario d), "seeding" of used modules to encourage secondary market development (Figure 1, scenario h), and existing regulatory policies such as a landfill ban¹¹ (Figure 1, scenario a) could also increase circularity. We also examine two existing business models of PV module manufacturers: extended producer responsibility and waste generator responsibility (Supplementary Figure 6).

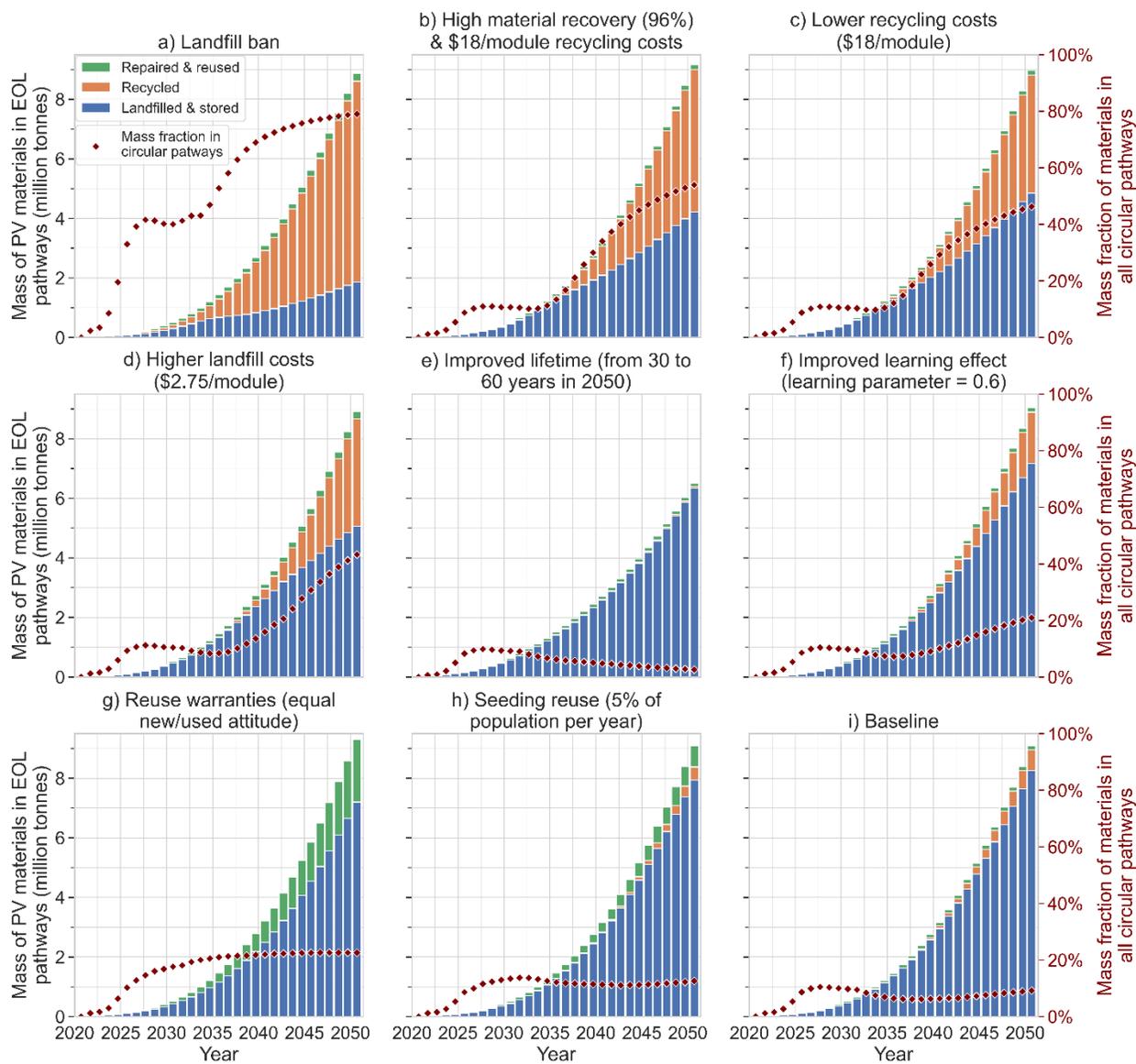


Figure 1: Various interventions could improve material circularity in the PV sector. Some interventions, including improved warranties (g) and seeding used modules (h), particularly boost module repair and reuse. Other interventions, such as lower initial recycling costs (c) and higher landfill costs (d), boost recycling. Reuse of EOL PV modules is limited by customer willingness to purchase used modules, which explains the circularity rate decline around 2035 in some scenarios, as EOL PV modules move from the reuse pathway to the landfill pathway. Although the simulations start in 2020, the generation of EOL PV modules is assumed to start from modules installed in 2000.

Exploring four interventions: lower recycling costs, higher material recovery, used module warranties, and used module seeding

One barrier to recycling EOL PV modules is lack of profitability^{11,26,30}. Module materials are difficult to separate and, for the most part, have low values³⁰. For example, silver accounts for half of the material value while representing less than 1% of module mass⁵. Thus, recycling costs are not offset by revenues from recovered materials in the current simple mechanical processes of glass and metals recyclers in the US, leading to recycling fees of \$25–\$30/module that PV owners or installers must bear in the absence of enhanced product responsibility or take-back programs²⁶. Some states, such as Maryland and Washington, have proposed tax incentives to overcome this issue^{31,32}.

Figure 2a shows the effect of varying initial (year 1) recycling costs in the ABM. The percentage of recycled EOL modules increases steeply with falling initial recycling costs before plateauing and reaching 73% recovery at zero cost. The plateau is due to several factors: 1) manufacturing waste is still landfilled, 2) for some PV owners, storage costs are null, so storage competes with free recycling, and 3) some cliques of agents reinforce each other into non-recycling behaviors through peer influence. Owing to the learning effect (Figure 2b), recycling is profitable by 2050 for each value of initial recycling costs below \$21/module (Figure 2a). With the current PV installed capacity and volumes of EOL modules, module recycling can still be considered in its infancy, and the learning effect likely will drive recycling costs down during 2020–2050. For instance, at an initial recycling cost of \$18/module (similar to the processing costs of high-recovery mechanical processes reported in the literature³⁰) instead of \$28/module in the baseline scenario, the recycling rate increases from 7.7% to 44% (or 4.0 million metric tons) in 2050 (Figure 1 and Supplementary Figure 3). With the learning effect this initial recycling cost enables recycling to be profitable by 2050 with a net income of \$0.09/kg. The material recycling rate is also higher when recycling processes recover more materials, e.g., with the Full Recovery End of Life Photovoltaic (FRELP) process. In this process, 94% of the silver and 97% of the silicon in c-Si PV modules are recovered²⁶, greatly enhancing the value of recovered materials (Figure 3 and Supplementary Figure 4).

When costs alone are included in the model, the recycling rate is always null as long as recycling is more expensive than landfilling (i.e., when initial recycling costs are above \$3/module)—see the “No social factors” line in Figure 2a. However, when social factors influencing PV owner decisions, such as peer influence and attitude toward recycling, are included the recycling rate increases with falling recycling costs. When social factors alone are included (the “No costs factors” line in Figure 2a), the recycling rate is overestimated or underestimated. Those results demonstrate the relevance of accounting for social aspects in the techno-economic analysis, because they may explain how and why a technology or behavior is adopted. In our case study, the positive effect of social factors on circularity when initial recycling costs are high shows the potential importance of nurturing early adopters of recycling behaviors who create a trend for other PV owners to follow.

One strategy to increase recycling is providing a subsidy until a recycling rate target is achieved. Our simulations indicate that a larger initial subsidy can be less costly than a smaller subsidy, because it engages more PV owners to recycle earlier (Figure 2c). Moreover, the learning effect supports recycling behaviors by lowering costs further, which leads to more PV owners adopting the recycling pathway. Overall, if the stream of EOL modules reaching recyclers keeps increasing (which is likely), the learning effect could spur profitable recycling without subsidies. In our simulations, a 20% recycling target can be reached earlier with an \$18/module subsidy (12 years) than with a \$10/module subsidy (18 years), limiting the period over which subsidies must be provided. The simulations show that a yearly recycled volume above 15,000 metric tons of EOL modules could make recycling profitable owing to the learning effect, a threshold value in line with the literature³³. High subsidies to encourage recycling and exploit the learning effect are a relevant strategy, but the results depend strongly on the presence of a sufficient learning effect. Thus, a subsidy program could benefit from establishing performance targets that verify continuous improvement of recycling processes, ensuring that recycling costs do not return to original levels once subsidies stop.

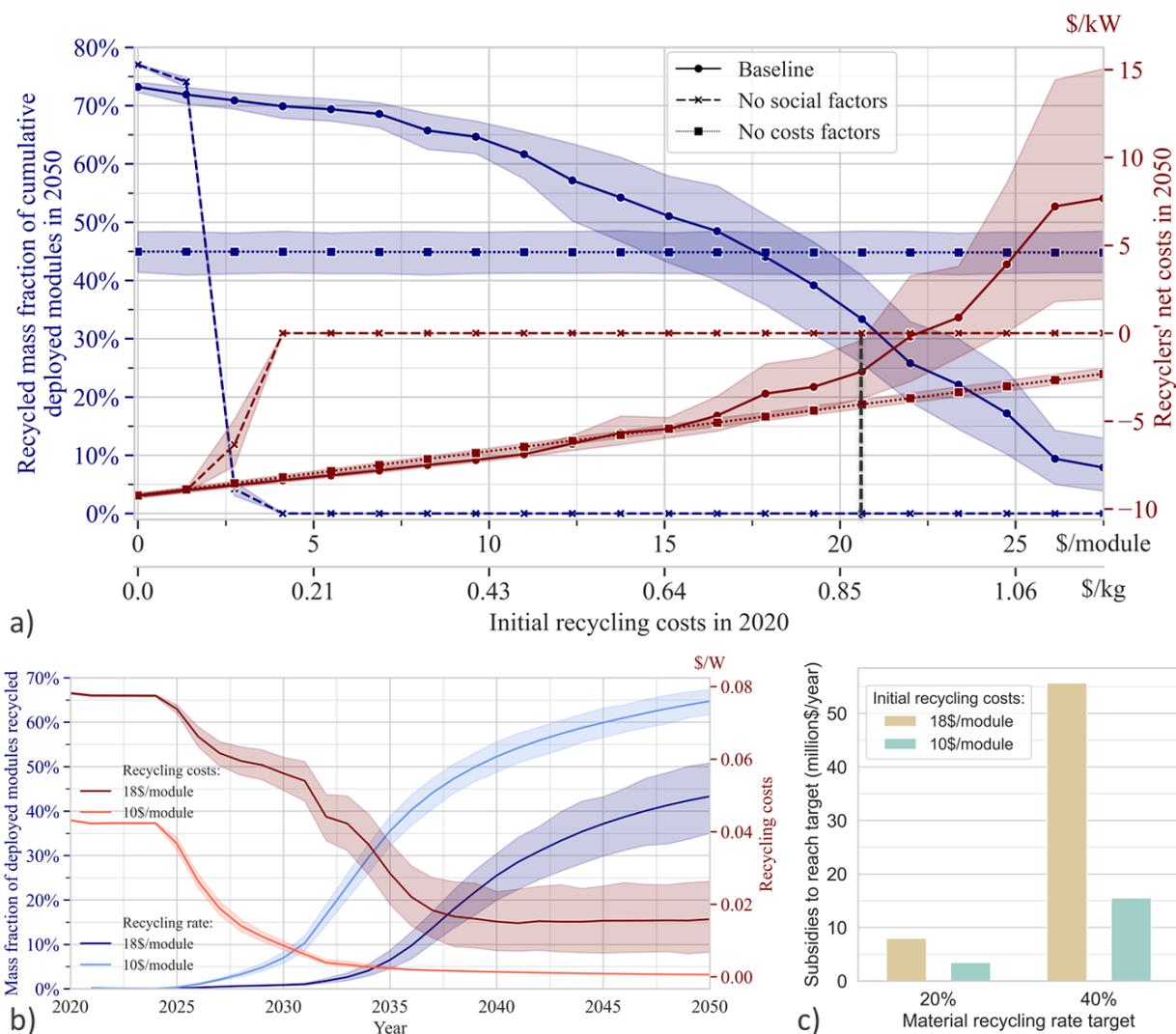


Figure 2: a) In the baseline scenario, the volume of materials recycled (cumulative total in 2050) quickly increases with falling initial recycling costs before reaching a plateau. Not accounting for economic factors (costs of recycling for PV owners) and social factors (attitude and peer influence) misrepresents the effect of lower initial recycling costs on the volume of materials recycled. Recycling is profitable (provides negative net costs, i.e., recycling costs minus value of recovered materials) by 2050 for initial recycling costs of \$21/module or less (black dashed line). Shaded areas represent 95% confidence intervals. b) Recycling costs decrease with the amount of PV modules being recycled. Shaded areas represent 95% confidence intervals. See Supplementary Figure 7 for a y-axis in \$/kg. c) High initial subsidies (initial recycling costs of \$10/module) boost recycling and help recyclers be profitable (due to the learning effect) more quickly than low subsidies (initial recycling costs of \$18/module), resulting in lower overall costs for the subsidy provider (\$16 million/year instead of \$56 million/year to reach a 40% recycling rate).

Recycling profitability could be increased through research and development in technologies that enable recovery of more valuable materials—such as silver, copper, and silicon—from EOL modules. High-recovery mechanical processes can enable higher material recovery, up to 97% of the total mass using the FREL process²⁶; however, in contrast with thermal recycling processes, such mechanical processes typically recover lower-quality materials with less value and usefulness than they had in the original module³. Figure 3a shows shares of modules in each EOL pathway and recycler net income assuming materials recovery fractions from the FREL process²⁶ and an initial recycling cost of \$18/module³⁰. FREL recovers 20% more materials per module than the baseline scenario and significantly increases recovered material value owing to silver and silicon recovery (Supplementary Table 1). This economic benefit is likely to weaken in the future, however, as innovation causes silver and silicon to constitute progressively smaller mass fractions in c-Si PV modules⁵; our analysis does not consider this trend because of the high associated uncertainty.

Recycler cumulative net income in 2050 increases from \$296 million in the simple mechanical process scenario to \$1.6 billion in the FREL scenario. Moreover, recycling becomes profitable earlier (2032 instead of 2037), with recycler net income reaching \$0.42/kg in 2050. Figure 3b shows the synergistic effect on recovered material value of lower initial recycling costs (which spur recycling among PV owners) and higher total material recovery fractions. Our simulations also show that some EOL modules are stored for a short period, leading to a small, relatively constant share of stored modules as PV owners and installers wait for cheaper and more accessible recycling options or the accumulation of quantities that are more economical to ship and recycle²⁶.

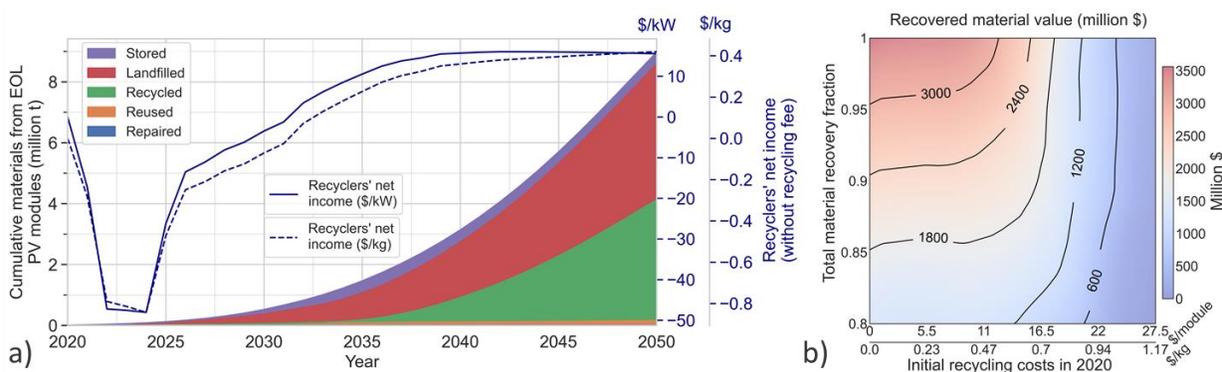


Figure 3: a) Cumulative materials from EOL PV modules and recycler net income assuming use of the FREL process and an initial recycling cost of \$18/module. The dip in recycler net income is due to initially unprofitable recycling. Still, with the low initial recycling cost and high recovery of materials (including silver and silicon), recycler cumulative net income reaches \$1.6 billion, and net income is \$0.42/kg, in 2050. b) Cumulative recovered material value in 2050. High materials recovery and low initial recycling costs have a synergistic effect on value generation, but the synergy diminishes as the

initial recycling costs is very high or very low. For instance, at an initial recycling cost of \$16/module, a 13% increase from an 80% material recovery fraction roughly doubles the recovered material value.

Improved warranties for used modules could promote secondary markets¹¹. The reuse rate increases from 1.2% to 23% (by 2.1 million metric tons) when assuming that warranties give PV owners an equivalent attitude toward used and new modules¹⁰ (Figure 1, scenario g, and Figure 4a). However, this assumption also decreases the recycling rate from 7.7% to less than 1%. Figure 4b shows that a 23% reuse rate only covers a small portion of projected PV demand. Even with an ambitious 89% reuse rate—set by removing all constraints to reuse except that modules can only be reused once—only a third of PV demand is met with used modules, highlighting the reuse strategy’s limitation. This result is explained by the projected growth of PV demand and the imperfect substitution of used modules for new modules (due to lower power efficiency and lifetime³⁴); see Supplementary Table 1. Once reused, modules still must be managed at the end of their second life, so developing other circular pathways such as recycling or lifetime extension is critical.

In practice, improved warranties may be insufficient to improve PV owner attitudes toward used modules, because other factors, such as safety concerns or aesthetic preferences, may intervene. Thus, other strategies to promote secondary markets should be considered. For instance, short-term “seeding”—providing free modules and installation to some PV owners—has proven to be an effective strategy³⁵ that could develop secondary markets for PV through the peer effect (Figure 1, scenario h). Such a seeding strategy applied to 5.0% of PV owners (i.e., at least 5.0% of PV owners have used modules each year) enhances the reuse rate from 1.2% to 6.9% but lowers the recycling rate from 7.7% to 4.7% (Figure 1 and Supplementary Figure 3). A similar strategy, in which 10% of PV owners pay a lower initial recycling fee (\$18/module), increases the material recycling rate to 21% (Supplementary Figure 8).

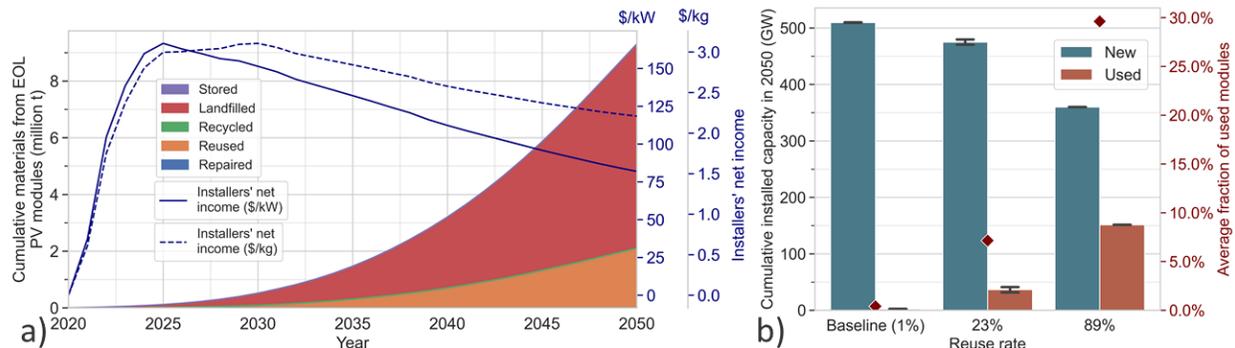


Figure 4: a) Cumulative materials from EOL PV modules and installer net income assuming improved warranties give PV owners an equivalent attitude toward used and new modules, showing substantial module reuse. Installer cumulative net income is \$3.5 billion, and net income is \$2.2/kg, in 2050.

After 2025, the net income per module decreases as innovation reduces PV module costs. b) Cumulative installed capacities of used and new modules in 2050 for various reuse rates obtained with our simulations; red diamonds represent the average fraction of used modules. In an ideal reuse case (89% reuse bars in the Figure), modules landfilled after their second life represent almost 10% of the cumulative EOL PV modules in 2050. Error bars represent 95% confidence intervals.

Sensitivity analysis and combined interventions

We use a ML metamodel of the ABM to conduct a variance-based sensitivity analysis and explore the ABM parameter space at higher speed. Figure 5 presents the first- and total-order Sobol indices for some parameters underlying the techno-economic and social interventions presented thus far. Initial recycling costs, landfill costs, and the learning effect are most important to the module circularity rate, with contributions of 48%, 33%, and 4% to the total variance in results, respectively (see Supplementary Table 3). Attitude toward used modules has a smaller but notable effect. Although some parameters present higher-order effects, the parameters rank similarly. However, the rankings change when examining output metrics other than the material circularity rate, such as the reuse rate or societal costs (see Supplementary Table 3 and Supplementary Figures 9–11). Finally, significant second-order interactions exist between initial recycling costs and other parameters (see Supplementary Table 4).

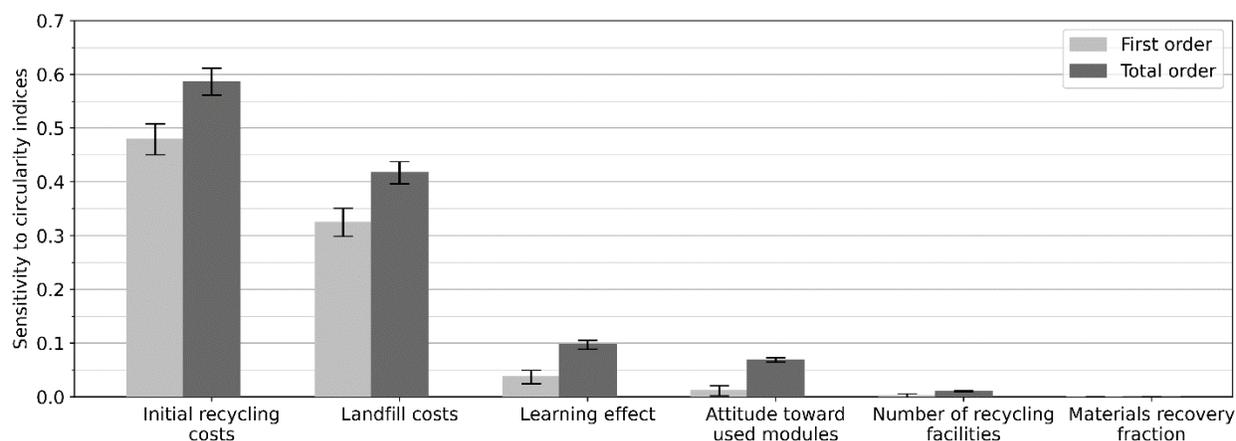


Figure 5: Parameter importance for EOL PV module circularity in the ABM, categorical parameters such as the landfill ban excluded. The y-axis shows the first- and total-order Sobol indices on the effect of a parameter on EOL PV module circularity. Error bars show 95% confidence intervals.

Figure 6 presents the interaction effects between initial recycling costs and four other parameters: landfill cost, attitude toward used modules, learning parameter, and number of recycling facilities. Increments of the learning parameter and landfill cost boost the effect of decreasing initial recycling costs on material circularity (Figure 6a and 6c). For instance, with initial recycling costs of \$10/module, raising the landfill

cost from \$1.38/module to \$2.76/module increases the material circularity rate from about 60% to 70% (Figure 6a). Because the reuse and recycling pathways compete, combining a more positive attitude toward used modules with lower recycling costs does not enhance the volume of PV materials diverted from landfills and storage (Figure 6b). Transportation costs are negligible compared with recycling costs, so having fewer facilities increases the material circularity rate slightly owing to an enhanced learning effect (Figure 6d). Finally, as with the sensitivity indices (Figure 5), the results are different when examining other output metrics (Supplementary Figures 12–13).

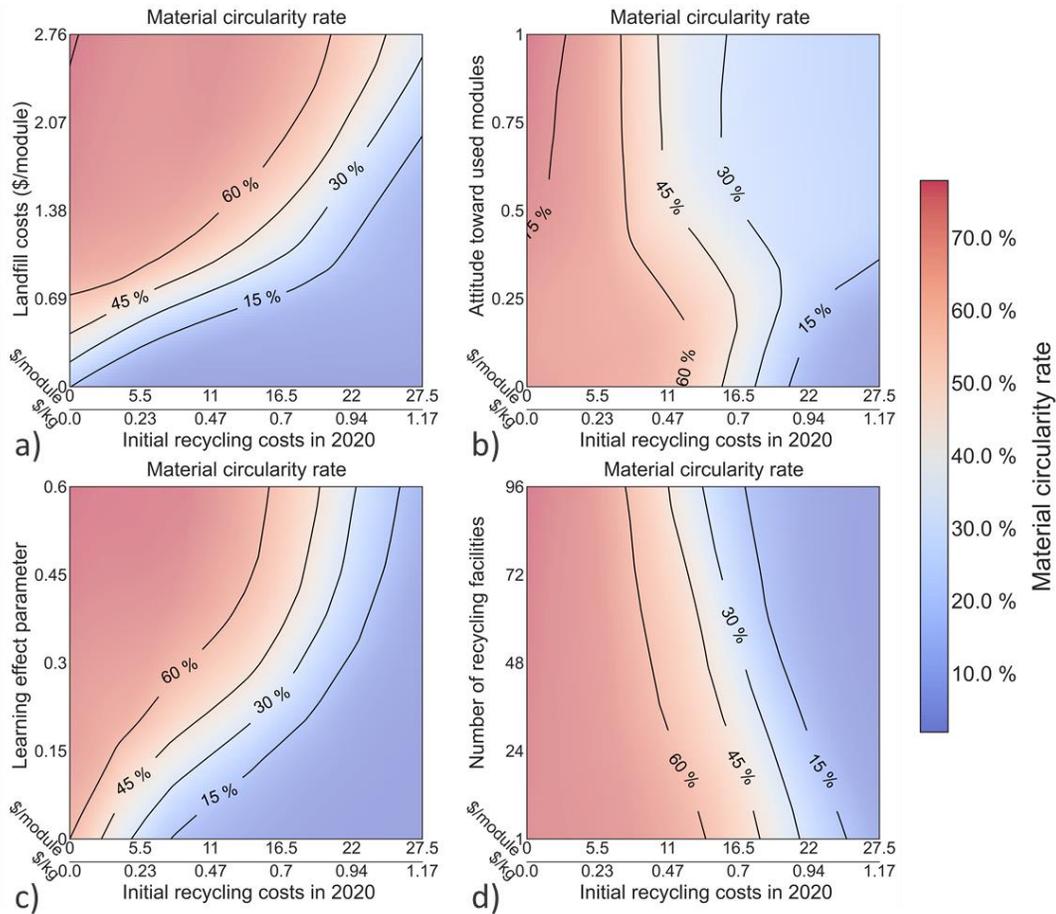


Figure 6: Fractions of PV module materials in circular pathways in 2050 as a function of the initial recycling costs (x-axis) and a) landfill costs, b) attitude toward used modules, c) learning effect parameter, and d) number of recycling facilities (y-axis).

Figure 6 also highlights that different intervention combinations may yield the same results (i.e., equifinality). For instance, initial recycling costs of \$18/module combined with landfill costs of \$2/module yield a 45% circularity rate, as do initial recycling costs of \$13/module combined with 48 recycling facilities. Using the ML metamodel, we designed an experiment to identify the parameter combinations maximizing circularity rate while minimizing societal costs (Supplementary Table 5).

Overall, combining low recycling costs, high landfill costs, and high learning effect yields the best result in the ABM, suggesting that combining interventions might be the most promising strategy to increase PV circularity at the lowest costs.

Limitations

Our results should be understood as estimates of how applying CE principles could affect EOL management of PV modules, instead of robust predictions. The ABM uses various sources as inputs, including some outside the PV sector (e.g., electronic waste literature) owing to the limited availability of primary data. Moreover, because some data variability is unknown, we approximate them using probability distributions, which adds uncertainty to the results (Supplementary Table 1). Although we use the TPB to better represent human decisions related to EOL management, factors not included in the theory may affect stakeholder decisions. In addition, we simplify stakeholders as constituting four broad categories (PV owners, installers, recyclers, and manufacturers); in the real world, the decisions of intermediary actors (e.g., brokers, insurers) may also affect PV circularity.

We limit the number of PV owner agents to a thousand, whereas more than 1 million real-world PV systems are in the US³⁶. Moreover, PV owners are not geographically characterized, albeit related through a social network. Although we use distributions to represent some geographical disparity, we distribute total installed PV capacity evenly between agents. Combining this ABM with a distributed PV model with better spatial resolution, such as the National Renewable Energy Laboratory's Distributed Generation Market Demand (dGen) model, could yield useful insights³⁷.

Implications

Our study yields several implications for PV circularity. First, our results suggest that CE strategies compete, in line with the literature³⁸. Thus, CE programs should be based on adoption rates for all circular pathways rather than focusing on one CE strategy. Second, for reuse to be effective, the used product supply must match demand, and therefore secondary markets must be mature³⁹. For example, only when PV owner attitudes toward used modules improve (e.g., through warranties) does demand grow and start substantially absorbing used module supplies. Improving reuse is critical from an energy perspective, because recycling destroys most of the embedded energy of products^{40,41}. However, owing to growing PV demand as well as the lower efficiency and lifetime of used modules, even a 100% reuse rate could not satisfy PV demand, so recycling must be developed in concert with reuse initiatives.

Our results also highlight the critical roles of the learning effect and total recovery fraction of materials to achieve profitable recycling (Figure 1), in line with existing literature³⁰. Interestingly, the storage pathway acts as a buffer, providing time for recycling processes to become more economical and ultimately

diverting some modules from landfills (Figure 3a). This result suggests that encouraging recycling may be particularly critical where storage space is more limited (e.g., Japan).

Exploiting the ABM approach, we extend the traditional techno-economic analysis to include social factors such as conformity to peers and general attitude toward a specific behavior. Accounting for attitude is especially relevant for PV, because households and businesses may be inclined to environmental protection and thus recycling^{42,43}. Our ABM can also be used to study interconnections and dynamics among different factors, as suggested by Lapko and colleagues³⁸.

Our results confirm the importance of factors such as the learning effect, research and development to reduce recycling costs, and public engagement³⁸. For manufacturers, recycling modules in a facility near the manufacturing line is a competitive advantage, because it makes manufacturing more resilient to supply restrictions and potentially facilitates recycling of manufacturing waste such as silicon kerf (Supplementary Figure 6). Recycling manufacturing waste is critical to improving circularity, because scrap materials are less contaminated and have compositions that are better known, compared with post-consumer materials⁴⁴.

Our results show that a landfill ban, such as the one in Washington State³¹, could increase PV circularity substantially (Figure 1, scenario a). However, legislation alone may be insufficient. Current European legislation, for instance, encourages mass recycling but not necessarily high-quality multi-materials recycling²⁶.

Our results finally show that high subsidies for a few years could be among the most efficient solutions for encouraging recycling. In contrast with Deng and colleagues, who found that landfill costs have the most potent effect, followed by recycling costs, we find that initial recycling costs have the most substantial effect, followed by landfill costs³⁰. This difference occurs because our model is more refined, including social factors and dynamic modeling of the learning effect.

In future work, the ABM could be used to study other scenarios, such as the effect of public information campaigns on recycling rates. Moreover, although a design-related intervention is briefly presented (Figure 1e), more scenarios related to the design stage, such as modules with different backsheet materials⁴⁵, could be explored. This novel approach combining ABM and ML could also be developed further to study the circularity of other technologies, such as consumer electronics, or to include environmental considerations.

3. Methods

Our ABM represents the main actors of the US PV sector that are involved in the transition to a more circular PV industry. Its objective is to find the techno-economic and social conditions that maximize materials circularity for EOL PV modules. The ABM's primary outputs are the mass volumes of modules reaching each EOL pathway (i.e., amounts that are reused, repaired, recycled, landfilled, or stored), the net revenue/cost for each CE actor, the value from recovered materials, and the number of years it takes to reach a specific objective. The overview, design concepts, and details (ODD) protocol is used to describe the ABM in this section⁴⁶, followed by details on the ML approach used to build a metamodel of the ABM and the sensitivity analysis method.

Overview

The purpose of the ABM is to study implementation of CE strategies within the PV industry and identify the conditions maximizing circularity. Four types of agents are defined: PV owners, installers, recyclers, and manufacturers. Agents of a specific type behave similarly but have heterogeneous characteristics represented by probability distributions (e.g., recyclers may have different recycling costs). Agents are related to each other according to a social network representing the real-world relationships among the CE actors. In the simulation, a time step represents a year. The start of the simulation is 2020; 30 time steps are chosen, because many installations will reach their EOL around 2050⁵.

At each time step, the ABM starts by modeling the cumulative amount of PV modules in use (i.e., the stocks) as well as the waste generated at their EOL. Then, agents make decisions about whether to comply with a particular CE strategy. The modeled CE strategies include repair, reuse (of a repaired/refurbished product), and recycle, and the two other options are landfill and store. Agent decisions are based on techno-economic factors—including technical feasibility, such as whether the modules can be repaired, and costs, such as landfill costs—and market factors (attitudes, social norms). The resulting volumes repaired, reused, recycled, landfilled, and stored change with each time step of the simulation. Supplementary Figure 1 presents an overview of the model.

Design concept

The ABM is designed in a modular fashion to ensure it can be used for different case studies; different types of agents may be defined and easily added to the model. Each agent type is defined as a Python module. In these modules, agent types are defined as a Python classes, and it follows that each agent is an instance of the class of its type. A Python model module contains all the user-defined inputs, activates the agents, and collects the outputs of the simulation. This modular structure is per the Mesa Python package⁴⁷. This package is used to facilitate the activation of the agents and set up batch runs of simulations. The NetworkX Python package is also used to build the social networks relating the agents⁴⁸.

Interactions between actors of the CE are captured at several levels in the ABM (that is, *within* agents of the same type and *between* agent types). First, because interactions between PV owners may influence their decisions regarding EOL management^{22,49,50}, they are accounted for in the model. Second, information flows between agents of different types. For instance, PV owners have access to recyclers' recycling costs, and installers access the amount of PV modules being sold by PV owners. As another example, manufacturers know the amounts of materials being recovered by recyclers and compute the economic benefits of using those materials rather than virgin materials.

The model also contains several stochastic elements. First, the Watts Strogatz algorithm, which is widely used to build small-world networks, requires to rewire each edge of a regular graph with a certain probability^{48,51,52}. Small-world networks are recognized as representing many real-world networks, including social networks⁵¹⁻⁵⁴. Second, some of the agents' characteristics are drawn from probability distributions to model their variability (e.g., recycling or landfill costs may be different across the US). Finally, the system's overall behavior emerges from the agents' interactions and decisions during the simulation.

Details

At the beginning of the simulation, the network of agents is created. The stocks of PV modules from 2000 to 2020 are reported in the ABM and divided among PV owner agents. We chose stocks from 2000 to 2020 to account for existing installed capacity, assuming that, before 2000, the cumulative installed capacity was negligible. From there, several sub-models are used to represent various dynamics of the hypothetical circular PV sector.

Environment

The environment of the ABM is the US. Various interventions may be enacted in the environment to see their effects. For instance, scenarios studying the implementation of a tax or a ban may be modeled as part of the environment agents evolve within.

Moreover, agents' interactions are dependent on a social network that represents the real-world relationships between the PV industry actors. In contrast with aggregated models, the ABM enables modeling of different social network structures and provides insights into the social network role in the overall behavior of the system⁵¹. Different network structures are adapted to different real-world situations. For instance, a fully connected network is more adapted to describing small groups and tight communities. For socio-technical systems such as the power grid or cities, the small-world or scale-free networks are more realistic^{51,53}. In the ABM, a small-world network is drawn using a rewiring probability and the average number of neighbors of 0.1 and 10, respectively. Those parameters are close to other works and real-world networks such as email communications^{51,55}.

Agents – PV owners

Owing to computational limitations, the number of PV owners was restricted to 1,000 agents. Although it limits the representativeness of the ABM, this number of agents enables capturing of network effects and the existing variability of PV owners (e.g., regarding landfill costs across the US or attitudes toward CE pathways). The PV owners make two decisions: 1) to purchase a new or a used product, and 2) to manage the EOL of their products.

Several processes are also occurring in the PV owners' module. First, the amount of product purchased each year is determined according to a piecewise function, following previous work⁵, and thus similar results for the projected installed capacity are obtained, although we only consider US c-Si PV modules. Values for the model's parameters can be found in Supplementary Table 1. Still following the literature, the efficiency growth of PV modules is accounted for with an exponential function⁵. Next, a Weibull function is used to generate the amount of PV modules of agent i reaching EOL at time t , $ELPV_i^t$ (Equation 1).

$$ELPV_i^t = \sum_t RPA_i^t \times (1 - e^{-(t/T)^\alpha}) \quad (1)$$

In the equation, T is the average lifetime of PV modules, α the shape factor (controlling the typical S shape of the Weibull curve), and RPA_i^t is the remaining amount of PV modules installed by agent i at time step t . The Weibull function is appropriate to model PV waste generation⁵.

The TPB⁵⁶ is used to model the PV owners' decisions to purchase used or new modules and the EOL management of those modules. The TPB stipulates that human behaviors are influenced by: 1) the attitude A individuals hold toward the behavior (i.e., how the behavior is perceived as favorable or unfavorable), 2) the subjective norm SN , which refers to the perceived social pressure to perform or not perform the behavior, and 3) the perceived behavioral control PBC , which relates to the perceived ease or difficulty of performing the behavior (Equation 2).

$$BI = w_A A + w_{SN} SN + w_{PBC} PBC \quad (2)$$

In the equation, BI is the intention to perform the behavior, and w_A , w_{SN} , and w_{PBC} are the weights of each factor in the overall decision. The TPB is often used in ABMs of socio-technical systems because it explains the process of individual decision making straightforwardly^{21,24,57} and has been applied in many waste-management ABMs^{21,22,24}. The theory explains consumers' decisions^{58,59} as well as decisions within companies^{13,60-62}. In our ABM, a score is attributed to each EOL pathway according to the TPB. The attitude level of each agent regarding CE pathways (repairing, reusing, and recycling) is normally distributed between 0 (negative attitude) and 1 (positive attitude). The attitude level toward linear

pathways (landfilling, storing) is simply assumed to be one minus the attitude held for CE pathways. Although this distribution of agents is rather simple when compared to the literature²¹, it is deemed sufficient for this exploratory analysis. Because the parameters of the truncated normal distribution were unknown, they were calibrated. Thus, an iterative process was undertaken to find the values that reproduce low recycling^{3,8} and reuse⁶³ rates as they represent today's situation. The second element of the TPB, the subjective norm SN_{ip}^t of agent i and pathway p at t , is defined as per Equation 3.

$$SN_{ip}^t = \sum_n \frac{Path_{np}^t}{N} \quad (3)$$

With $Path_{np}^t$ being one if agent i 's neighbor n has selected the path p and zero otherwise, and N being the total number of neighbors of agent i . Thus, the subjective norm takes values between zero (no peer pressure) and one (maximum peer pressure). While in the ABM neighbors designate nodes that share an edge in the small-world network, they may represent various relationships among PV owners in the real world (e.g., friends, family, coworkers, and actual neighbors). The third element of the TPB, the perceived behavioral control PBC_{ip}^t of agent i and pathway p at t , is given by Equation 4:

$$PBC_{ip}^t = -\max\left(0; \frac{Cost_{ip}^t}{|\max\{Cost_{ip}^t \forall p\}|}\right) \quad (4)$$

Where $Cost_{ip}^t$ is the cost of choosing the pathway p at t for agent i . Finally, the behavioral intention BI_{ip}^t of agent i for pathway p at t is defined by Equation 5

$$BI_{ip}^t = w_A A_{ip}^t + w_{SN} SN_{ip}^t + w_{PBC} PBC_{ip}^t \quad (5)$$

In Equation 5, the values for the coefficients w_A , w_{SN} , and w_{PBC} are taken from an existing meta-analysis on factors affecting EOL management decisions⁵⁰. Even though we use a meta-analysis, the coefficients' values are uncertain and, thus, could alternatively be calibrated. However, the lack of empirical data prevents us from conducting such extensive calibration. The agent then selects the EOL pathway with the highest score (and the amount of EOL modules $ELPV_i^t$ is recorded as following the selected pathway for further use by other agents and the output metrics).

The TPB is also used to model the purchase decision, similar to how the EOL decision is modeled. Two options are represented in this ABM, the purchase of a new or a used module (see Supplementary Figure 14). Another meta-analysis is used to determine the TPB coefficient values for the purchase decision⁵⁸. The TPB may be interpreted in terms of material efficiency potentials. If one defines w_A and w_{SN} to be 0, the techno-economic potentials of the recycling, repairing, and reusing CE strategies may be studied on their own. Otherwise, the social factors of the model (the subjective norm and attitude) may be added, enabling study of the achievable (or market) potential of material efficiency¹⁵.

Agents – Installers

Installers are the second type of agent. In the PV sector, installers may be in charge of collecting EOL PV modules and eventually sorting them before selling them on the secondary market⁶⁴. They may also repair failed modules if PV owners opt for that EOL pathway. If there is insufficient demand for used modules or if they are too damaged or cost too much to be repaired (Equations 6-7), installers send them to a recycler or landfill, or they store them until another decision is made depending on the cheapest decision at the time of the simulation (using Equation 4). It is assumed in this model that handling used PV modules always bears the same repair costs (whether modules are repaired directly for PV owners or sold as used products) regardless of possible damage to the EOL modules.

$$V_j^t = \frac{RR \times (\sum_i V_i^t + \sum_k V_k^t)}{\sum_j} \text{ for } i \text{ and } k \text{ such that } RC_i^t \leq RP_j^t \text{ and } RC_k^t \leq RP_j^t \quad (6)$$

$$RA_j^t = \begin{cases} V_j^t & \text{if } \sum_j V_j^t \leq \sum_i DU_i^t \text{ for } i \text{ such as } PU_i^t = 1 \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

In the equations, V_j^t is the volume of modules available for sale on the secondary market by installer j . Next, RR is the module repair rate, V_i^t and V_k^t are the volume of modules flowing from the PV owner i and recycler k at time t , respectively, RC_i^t and RC_k^t are the repair costs of modules from PV owner i and recycler k at time t , respectively, and RP_j^t is the price at which agent j is selling the used modules on the secondary market at time t . Finally, RA_j^t is the amount of used modules handled by installer j that is sold on the secondary market at time t ; it depends on the demand for used modules from PV owners ($\sum_i DU_i^t$). In the equation, PU_i^t is a boolean being one when the PV owner i has decided to purchase a used module at time t and zero otherwise. Installers also improve their repair processes owing to the learning effect, thus decreasing repair costs. The learning effect can be characterized by several mechanisms, such as technology advancement, increased labor productivity, economies of scale, and improved material and energy efficiency²⁸. As the volume of EOL PV modules dealt by an installer increases, at least three of these mechanisms may apply: increased labor productivity, economies of scale, and energy efficiency. In the ABM, the learning effect is modeled as a function of the repaired volume, following the literature²⁸.

Agents – Recyclers

Recycler agents are similar to installers in two ways. First, they may take on the responsibility of sorting EOL PV modules that can be sold on secondary markets (with those modules then flowing to installers); this behavior was assessed via interviews with a US recycler⁶⁵. Second, recyclers improve their recycling processes in the model, simulating the learning effect. Another recycler role is to recover materials from EOL PV modules. In the ABM, this is simply modeled from the material recovery rates of a given

recycling process (e.g., simple mechanical processes or the FREL process²⁶), the fractions of materials that constitute PV modules, and the volume of modules being recycled. In the ABM, PV owners pay a fee to recycle EOL PV modules, while manufacturers buy recycled materials at market prices. With current US recycling processes, revenue from recovered materials is insufficient to cover recycling costs²⁶.

Agents – Manufacturers

Manufacturer agents purchase recovered materials from recyclers. The avoided costs from using recovered rather than virgin materials can be computed within the model based on their respective values. For instance, the price of aluminum scrap is often about 60% of the price of virgin aluminum⁶⁶, which brings profits for manufacturers that use aluminum.

Validation

We applied four validation techniques to ensure the quality of the results produced by the model: theory validation, data validation, model output validation, and face validation⁶⁷. First, regarding theory validation, only empirically validated models were used (e.g., TPB). Next, for the baseline scenario, empirical data were mostly used; when parameters were unknown, they were calibrated^{3,5,8,63}. Then, the cumulative installed capacity and the mass of EOL PV modules generated during the 2020 to 2050 period were validated with the literature⁵ (Supplementary Figure 5). Finally, the results of the ABM went through an internal revision process with ABM and PV experts to ensure the model was behaving in a meaningful way, and extreme scenarios were also studied (see Supplementary Table 6).

Machine-learning metamodel and sensitivity analysis

The combination of ABM and ML has recently gained attention owing to the complementarity of the two approaches⁶⁸. These methods can be combined in two ways: ML can generate agent behavioral rules from data³⁵, and an ABM can be explored in depth (i.e., varying the ABM inputs to examine a wide range of possible outputs) by building a ML metamodel (i.e., a model of a model) that avoids computationally intensive simulations and saves time⁶⁹. Because of the exploratory nature of this work, we use the second approach in this study. Following Vadhati and colleagues, we built a ML metamodel of the ABM described above⁶⁹. Using the Scikit-learn Python library⁷⁰, we constructed different ML models using different combinations of hyperparameters. In our study, all features (input data) and output data are known in the dataset generated by the ABM; thus, supervised ML is used.

In this study, the training dataset is generated with the ABM. To produce the dataset that best represents the behavior space of our model while limiting the required number of simulations, we use a quasi-Monte-Carlo approach. First, the range of each parameter to vary in the quasi-Monte-Carlo simulations is defined. For some parameters, it is merely their minimum and maximum possible values (e.g., for ratios).

For parameters without theoretical bounds, realistic ranges are defined according to the literature. For landfill costs, for instance, the minimum value is set to zero, while the maximum value is set to twice the average value of the baseline scenario; it seems unrealistic that landfill costs could be higher than that based on current trends²⁷. A similar logic is applied to other parameters (Supplementary Table 5). Next, the method from Saltelli and colleagues is used to generate the Sobol sequences of parameter value combinations⁷¹. Sobol sequences aim to approximate the model's behavior within the parameter space by attempting to cover as much of the parameter space as possible as quickly (with the fewest samples) as possible. This is one of the highest-performing methods (e.g., compared with the Latin hypercube design) regarding the quality of results obtained as a function of computational time, and it is often used to build metamodels^{72,73}. Thus, using the SALib Python library⁷⁴, 2,800 parameter value combinations are generated, to which we add the baseline parameter value combination as well as variants of the baseline varying each parameter to its lower and upper bound (to include extreme cases in our dataset). In total, 2,810 parameter value combinations are run a total of 6 times (to account for the stochasticity of the model), amounting to 16,860 simulations.

Next, we iterate 10-fold cross-validation, varying the ML algorithm, its hyperparameters, and the output metric considered in the dataset. We keep the multilayer perceptron regressor algorithm, which yields a good compromise between computation time and a high coefficient of determination in all output metrics (Supplementary Table 7). Once trained, the metamodel is used to predict the outputs of parameter value combinations not run with the ABM. The SALib library is finally used to conduct a variance-based (Sobol) sensitivity analysis and thus measure the uncertainty of model outputs that can be accounted for by changes in model inputs. We use the Sobol method because of its ability to evaluate interaction effects and the low risk that dependencies exist between the parameters of our ABM. Moreover, we compare results from the variance-based sensitivity analysis with results from a moment-independent sensitivity analysis to confirm rankings of parameters (Supplementary Table 3). Because of the use of the ML metamodel, results from Figures 3b, 5, and 6, Supplementary Tables 3–5, and Supplementary Figures 9–13 are approximations of the ABM's results.

4. Data availability

The authors declare that the data supporting the findings of this study are available within the paper and its supplementary information files.

5. Code availability

The source code for the model developed in this study can be accessed on:

<https://github.com/NREL/ABSiCE>

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