

# Ranking Eco-Innovations to Enable a Sustainable Circular Economy with Net-Zero Emissions

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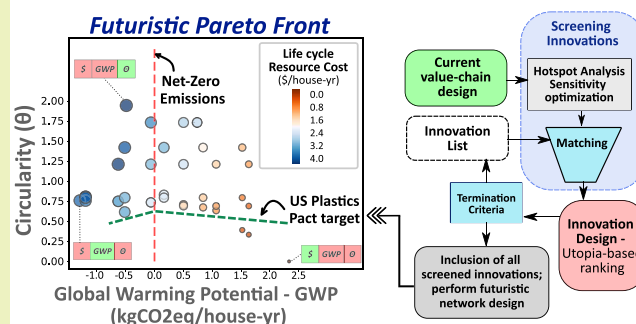
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**ABSTRACT:** The urgency of action toward mitigating climate change and reducing material leakage into the environment is inspiring a plethora of innovative technologies, supply chains, and policy actions. These are targeted toward reducing greenhouse gas emissions, natural resource uptake, and decoupling technological systems from fossil-based linear economies using circularity strategies. Industrial and governmental stakeholders are keen to rank these proposed eco-innovations and emerging alternatives based on their scope of contributing to a sustainable and circular economy to meet global warming curtailment and pollution mitigation targets. We describe a novel methodological framework that relies on a multiobjective optimization of cradle-to-cradle life-cycle pathways to screen from a large database of conceptual eco-innovations and rank them based on their potential for establishing a Sustainable Circular Economy (SCE). This methodology is implemented for a motivating case study to evaluate numerous packaging eco-innovations based on their improvement potential and readiness for adoption within the grocery bags value-chain network. It is demonstrated that a preliminary screening step identifies the 10 most promising eco-innovations from a large superset of alternatives, which if developed and adopted can help transition the value chain to a future scenario with net-zero emissions and adherence to the recycled and renewable-content targets set by the United States Plastics pact but at a higher cost.

**KEYWORDS:** Sustainable circular economy, Environmental targets, Net-zero emissions, Eco-innovations, Life cycle assessment, Multi-objective optimization

## Methodology to guide innovations for Net-Zero + Circularity



## INTRODUCTION

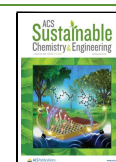
Governments and corporations from around the globe are making pledges to achieve net-zero emissions to limit climate change and plastic pollution for as early as 2030.<sup>1–3</sup> Such pledges include: (a) Paris agreement between countries to reduce greenhouse gas emissions for limiting global temperature increase to 2 °C by 2100;<sup>4</sup> (b) Carbon neutrality targets by corporations to curtail CO<sub>2</sub> emissions to net-zero (e.g., Amazon by 2040, Dow Chemical by 2050, Microsoft by 2030, etc.);<sup>5,6</sup> (c) US plastics pact targets to curtail plastic pollution by ensuring 30% recycled, responsibly sourced, or biobased content, etc. While such pledges raise global hopes for keeping human activities within planetary boundaries,<sup>7</sup> meeting these pledges is a truly formidable challenge.<sup>5,8</sup> In particular, these pledged targets must be met sustainably, which means they must ensure that the pledging entity maintains economic feasibility and that their activities are socially desirable and ecologically viable during and after their transition to the pledged goals. Innovations and novel alternatives within current value-chain networks are expected to be essential for meeting the pledges.<sup>9,10</sup> Ranging from polymers and plastics to energy systems and semiconductors, a large number of

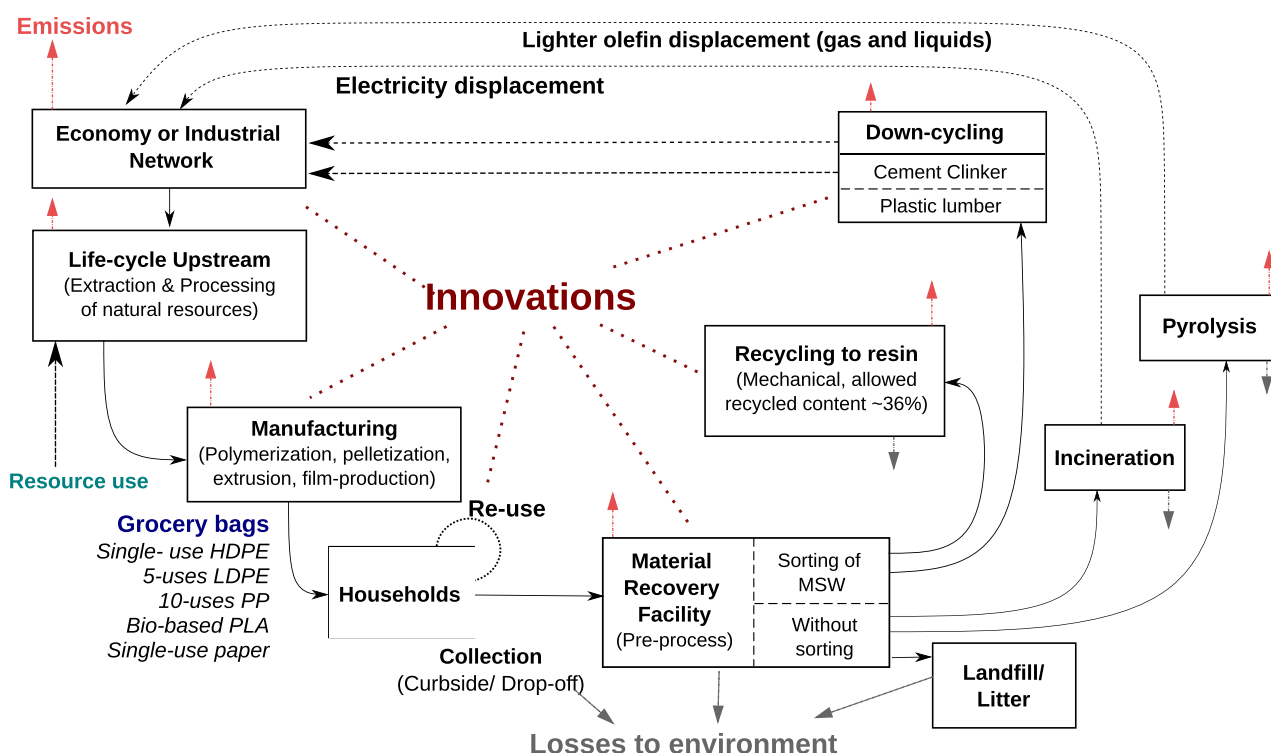
innovations and emerging technologies are being developed by academicians, entrepreneurs, and corporate research and development (R&D) alike. Owing to the imminent perils of global warming and ecosystem degradation, a large fraction of these innovations (hereby referred to as “eco-innovations”<sup>11</sup>) are targeted toward sustainable development and mitigation of environmental impacts. However, not all proposed eco-innovations are likely to be holistically sustainable due to shifting impacts beyond a narrow system boundary, nor can they all be expected to reduce trade-offs that commonly occur between emission reduction, increasing circularity, and profitability.<sup>12,13</sup> Therefore, technology and policy forecasting are needed to quantitatively estimate the implications of adoption of these innovations before investments are made.<sup>14</sup> Additionally, due to an immeasurably large number of proposed

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**Figure 1.** Carrier bags' value-chain network considered for the case study. Solid arrows indicate cradle-to-cradle flows of the primary products, whereas dashed arrows indicate down-cycled flows. Dotted lines indicate the presence of eco-innovations in various value-chain activities. The continuous variables include product ratios in various streams, split fraction of streams at the material recovery facility, etc.

innovations and the urgency of action, it is imperative to evaluate them in a systematic and efficient manner while being holistic and fair in comparison. Developing a methodological framework to do so is the objective of this work.

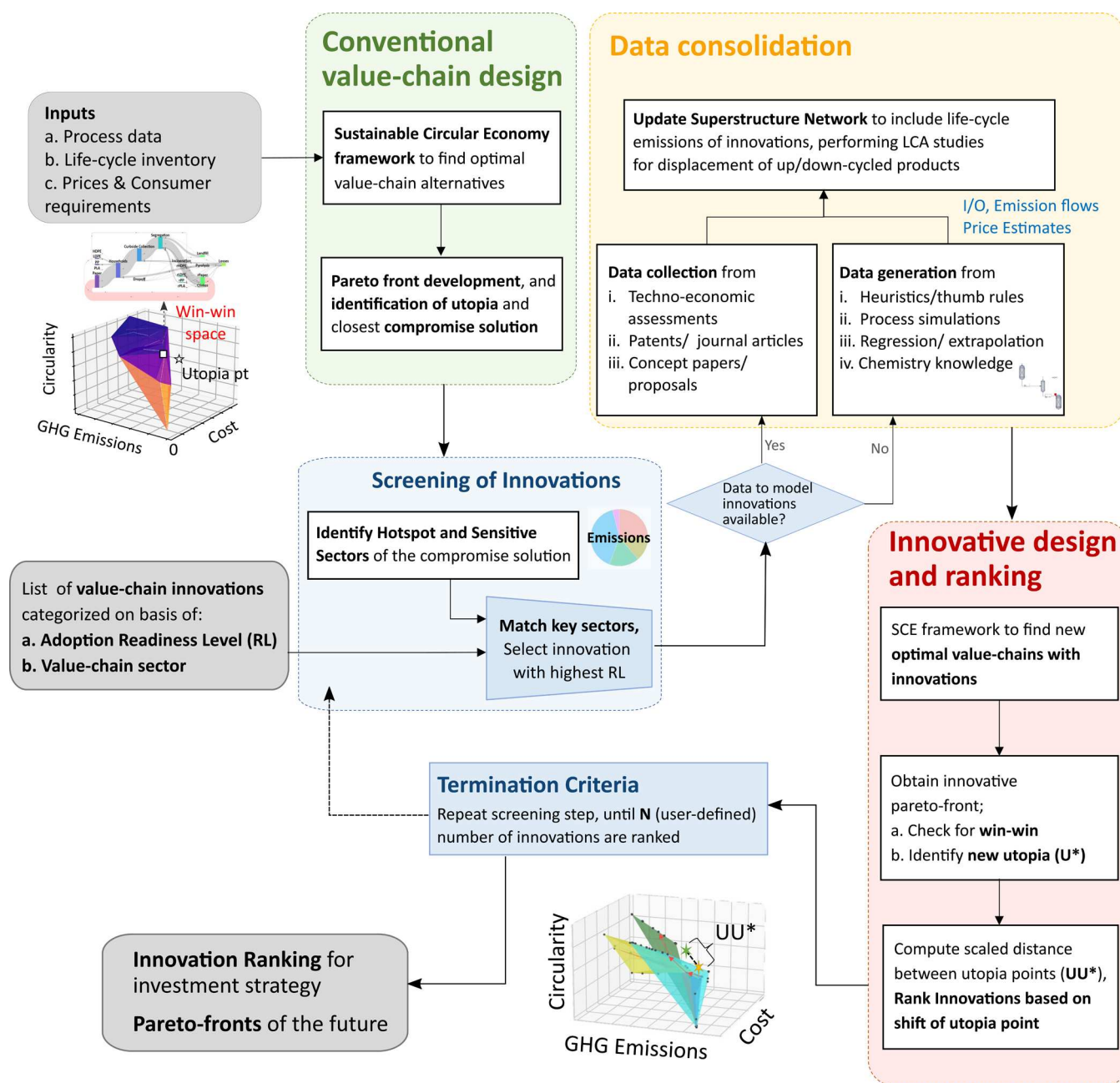
There have been many published efforts to model, assess, develop, and design eco-innovations in the past. These efforts are characterized by Hazarika and Zhang (2019)<sup>15</sup> into one of three levels, namely, microlevel (concerning management and organizations), mesolevel (related to networks and markets), and macrolevel (socio-economic and policy targeted). The authors also find that there are relatively few quantitative studies and frameworks to study eco-innovations within the meso-level. Xavier et al. (2017)<sup>16</sup> have conducted an exhaustive literature review of eco-innovation models and classified them into six types based on research areas and identified the gaps in each area. They identify that, within the “innovation strategy” and “industrial ecology” domains, methods are predominantly qualitative or experimental, and a more quantifiable basis is needed to build organizational and policy-based strategies to propagate eco-innovations selectively. These studies inspire us to focus on modeling life-cycle network implications of eco-innovations at the meso-level in our proposed framework.

Life-cycle assessment (LCA) has also been used to assess eco-innovations, but Motta et al. (2018) review recent literature and conclude that this application of LCA is still in the initial phase.<sup>17</sup> There is a huge scope to use LCA for guiding eco-innovations because it lends a “systems” view for holistic analysis of these emerging approaches.<sup>18</sup> However, most published work on applying LCA for eco-innovations has a product eco-design perspective,<sup>19</sup> making it difficult to evaluate a large set of alternatives and avoid shifting impacts outside the system boundary. Recent methodological develop-

ments such as anticipatory and prospective LCA focus on calculating the environmental impact of emerging technologies and associated uncertainty due to future implementations.<sup>20,21</sup>

While these are extremely useful to perform a deeper analysis of singular eco-innovations, the need of the hour is to systematically compare many such proposed eco-innovations and select the best options. Given the computational load of analyzing each eco-innovation, its interaction with steps in the life cycle, and their effect on various objectives, a systematic framework with efficient methods can prove to be extremely useful in performing faster screening and ranking of eco-innovations. In addition, the presence of trade-offs between environmental and economic objectives reinforces the need for employing systems engineering and multiobjective optimization to achieve win-win solutions through eco-innovations.

Many recently proposed eco-innovations aim to establish a Sustainable Circular Economy (SCE), which requires restoration of material and energy within the value chain to reduce waste and limit emissions to the environment. Thus, to identify eco-innovations that can successfully establish SCE, they must be evaluated for sustainability in terms of cradle-to-cradle life-cycle impact, economics of operation, and circularity of reformed value chains before their adoption. In this work, we develop a novel methodology to (a) screen innovations from a compiled list based on hotspots in the current life-cycle and (b) rank them based on the potential ability to improve SCE and reduce trade-offs. This method is able to determine which eco-innovations to invest in, while considering life-cycle impact and circularity simultaneously using multiobjective optimization. It also helps refine the search space and reduce the computational load of evaluating all innovations based on hotspots in current value chains and activities with the highest potential of improving SCE. The outcome of the proposed



**Figure 2.** Methodology for screening and ranking innovations, with each box header being a subsection header within the [Methods](#) section.

methodology is a cumulative ranking based on a novel “utopia” shift criterion to evaluate win-win opportunities and reduce the trade-off between objectives. We go a step further and allow the user to find an ideal combination of eco-innovations for investment, in a futuristic scenario wherein all the screened eco-innovations are adoptable. While the proposed method provides a quantitative basis for prioritizing future investment, large-scale adoption of these new technologies should be undertaken only after evaluating the impact of novel technologies and life-cycles on local and global ecological carrying capacity<sup>22,23</sup> of several ecosystem goods and services. Nevertheless, the proposed methodology can be used by private corporations, governments, and venture capital firms for eco-innovation portfolio management, thereby allowing development of a roadmap to meet Sustainability and Circularity targets in an optimal way. This method can

therefore advance the organization’s sustainability goals such as net-zero emissions, circularity, and decarbonization by providing a basis for future sustainability transitions. For demonstration of the proposed methodology, we apply the SCE framework to a motivating example: the grocery bags value-chain and eco-innovations proposed for the plastics packaging industry. Needed innovations and alternatives could be technological, ecological, and economic, but in this work, our focus is on technological options. However, if the life-cycle inventory for the ecological and economic eco-innovations is available, the methodology can include those as well.

The rest of this paper is organized as follows. The next section describes the motivating example used to demonstrate the novel method. This is followed by the methodology section, which describes the approach and the steps required to screen and rank innovations in a stepwise manner, including a



novel ranking criterion based on win-win, readiness for adoption, and trade-off reduction between sustainability, circularity, and cost. Ultimately, the [Results and Discussion sections](#) illustrate the improvement in SCE that can be brought out by the screened eco-innovations in the grocery bags value chain. The [Conclusion section](#) describes the general applicability of the methodology and its potential use for facilitating vital sustainability transitions through eco-innovations.

## MOTIVATING EXAMPLE: GROCERY BAGS

While the approach proposed in this paper is general and applicable to value-chains of any product or service, we demonstrate the proposed methodology using a motivating example of the grocery bags value chain shown in [Figure 1](#). This section is devoted to a description of the value chain and eco-innovations from the plastics packaging industry that are screened and ranked using the proposed methodology.

The alternative pathways in the carrier bags' value chain stem from type of bag to be manufactured, collection method, and decisions at the material recovery facility. As a result of these options, there are 120-odd pathways and an infinite number of combinations due to continuous variables arising from mixed streams and segregation. These alternative pathways form the "superstructure" network of interest. A superstructure is a large space of structural alternatives,<sup>24</sup> each corresponding to a feasible solution pathway. For our carrier bags motivating example, the superstructure is shown in [Figure 1](#). The manufacturing sector in the network takes in inputs from the life-cycle upstream and can produce five types of bags,<sup>25</sup> each made of a different raw material and having unique reusability and volume carrying capacity. These bags can be used by a single representative household, which disposes its mixed household waste either through curbside collection or drop-off to a center. This waste is then transported to a material recovery facility (MRF). At the MRF, the waste can either be segregated and mechanically recycled to substitute virgin plastic or paper or down-cycled to lumber or cement filler. The mixed waste can also be directly landfilled, incinerated to produce electricity, or pyrolyzed to fuel. All these alternative value-chain pathways and linked upstream life cycles form the cradle-to-cradle superstructure network shown in [Figure 1](#).

## METHODS

Utilizing the motivating example stated in the previous section, this manuscript develops a methodology to accomplish the following tasks:

- Optimize the conventional value chain.<sup>26,27</sup>
- Find hotspots in the value chain and activities to which the objectives are most sensitive to. These form the target sectors for screening promising eco-innovations.<sup>27</sup>
- Short-list conceptual eco-innovations based on sector and readiness for adoption.
- Model these innovations for inclusion in the superstructure network.
- Optimize a new superstructure network to determine the benefits of innovation.
- Rank several short-listed (or screened) eco-innovations.

While the first two steps can be performed using frameworks developed in previous work,<sup>26,27</sup> the remaining steps are aimed toward screening and ranking eco-innovations, and they are novel contributions. The proposed methodology has been summarized in

[Figure 2](#). Details about each step in this figure are described in the rest of this section.

**Conventional Value-Chain Design.** The first step of the methodology is to explore the currently available alternatives in the value-chain network to find the optimal combination of these alternatives to achieve a Sustainable Circular Economy. This includes finding the trade-offs between optimal solutions for minimum emissions, cost, and maximum circularity. These steps are shown in the green box in [Figure 2](#). Ultimately, the optimal solutions generated from the SCE framework will be used to find hotspots and the largest contributors of negative impacts under currently existing technology and policy constraints. The multiobjective optimization method used for this purpose has been described and applied in Thakker and Bakshi (2021a,b). However, the next few subsections will describe this in brief.

**Sustainable Circular Economy Framework for Value-Chain Design.** The Sustainable Circular Economy (SCE) framework is a life-cycle design framework that uses systems engineering and optimization to identify optimal value-chain pathways from a "superstructure" network of alternatives.<sup>26</sup> This network is built using life-cycle inventory data and contains inputs, outputs, resource-use, and emissions from value-chain activities. In the LCA literature, such a network is mathematically represented in the form of technology and intervention matrices. However, LCA deals with matrices that have full rank, meaning it can only assess individual pathways but is unable to identify optimal designs and combinations. Additionally, LCA can only evaluate circularity options using discrete amounts of products that displace the upstream lifecycle, thereby leading to subjective bias in scenario generation and large computations. To accommodate the need for generating circular designs, the SCE framework makes a few modifications to the computational structure of LCA using mathematical programming, which allows us to have a choice between multiple alternatives at the upstream and downstream of several activities. Ultimately, this choice is viewed as a "degree-of-freedom" and is exploited using optimization to find the "best" possible choice (or decision variable) for a carefully formulated objective.

Since the SCE framework relies on LCA, it requires declaration of few model parameters and attributes, including Goals and Scope, System boundary, and Impact Assessment method,<sup>28</sup> which have been described in section S1.1. of the [Supporting Information](#) document. Subsequently, an optimization formulation needs to be prepared as per the requirements of the SCE framework,<sup>26</sup> which involves building a superstructure matrix using the computational structure of LCA and addition of constraints corresponding to consumer demand, material-energy balances, and other governing equations for stream compositions. This has been summarized from Thakker and Bakshi (2021a)<sup>26</sup> briefly in section S1.2 of the [Supporting Information](#). Due to the presence of multiple stakeholders within a value chain, the SCE design has to be solved as a multiobjective problem with objectives falling into three major domains: Sustainability, Circularity, and Economics. While certain stakeholders aim to achieve environmental sustainability by minimizing life-cycle impact, others want to maximize restoration of value in the network through circularity, and the rest to minimize cost of natural resources from the lifecycle. Therefore, the objectives used for the grocery bags value chain from the respective domains are (1) Sustainability - Global Warming Potential (GWP) through greenhouse gases, (2) Circularity -  $\theta$  defined as the monetary value of circular products divided by manufacturing costs, and (3) Economics - Cost of Natural Resources used in the Life-Cycle (LCC). The mathematical formulation of these has been stated in eqs 2-(4) of Thakker and Bakshi (2021b)<sup>27</sup> and discussed in [section S1.3](#).

**Pareto-Front Development, and Identification of Utopia Point.** Optimizing the superstructure network for each objective is likely to give a unique solution. This indicates the presence of trade-offs between the SCE objectives, namely, environmental impact, circularity, and cost of natural resources. This trade-off can be quantified using multiobjective optimization techniques such as augmented epsilon-constraint method (AUGMECON)<sup>29</sup> to generate

a three-dimensional (3-D) Pareto-front plotted on the objective function space. These Pareto-fronts cover the win-win-lose (or compromise) solutions, which means that the choice of a particular solution over another in the Pareto-optimal set (to improve one objective) cannot happen without compromising on the other objective. This Pareto-optimal solution therefore indicates the best possible solutions from the superstructure network. On one side of the Pareto-front lies the suboptimal space, whereas on the other lies the infeasible (or win-win) space. Within the infeasible space, the “utopia” point can be traced from the optimal values of all objective functions that can be achieved independently. In order to obtain solutions in the win-win space, one has to modify (or improve) the superstructure network by adding better alternatives, such as emerging technologies and innovations. Therefore, for this application, we claim that the name of “infeasible” space can be recoined to “innovation” space. These aspects of Pareto-front exploration are critical for this method.

**SCE Optimal Value Chains for the Grocery Bags Example.** The SCE framework, when applied to the grocery bags example, yields optimal value-chain combinations for the objectives, (i) Global Warming Potential (GWP), (ii) Life Cycle Cost of Natural Resources (LCC), and (iii) Economic Circularity ( $\theta$ ). While these value-chain pathways are elaborated in Thakker and Bakshi (2021b),<sup>27</sup> the results can be summarized as follows: the minimum LCC optimum prefers reusable polyethylene (PE) bags being consumed and littered to the environment (avoiding the cost of collection and processing), whereas minimum GWP optimal value chain involves consuming the same reusable PE bags, mechanically recycling them up to permissible limits, and using the rest for producing plastic lumber. On the other hand, maximum economic circularity is obtained for single-use PE bags being mechanically recycled and incinerated to generate electricity. The larger volumes of single-use waste make circular flows more profitable, however, leading to higher GWP and LCC.

These unique optimal value-chain solutions indicate the scope of improvement in the three SCE objectives and the presence of trade-offs between them, which is quantified and measured using Pareto-fronts and the utopia point (UU\*) in the objective space, as described in the previous subsection and depicted in Figure S1 of the [Supporting Information](#).

**Screening of Innovations.** The next step of this methodology, as shown to succeed the green box in [Figure 2](#), is to screen innovations from a large conceptual list based on (a) whether they address key hotspots and sensitive sectors and (b) their respective readiness for adoption.

**Identify Hotspot and Sensitive Sectors.** Since modeling conceptual eco-innovations requires considerable effort and time, it is not possible to include “all” of the proposed innovations in the superstructure network simultaneously. The innovations must be screened based on a vetting criterion before modeling. We propose that this vetting criterion should consider the hotspot and sensitive sectors from the conventional value-chain design, performed in the previous section.

The highest contributing activities of the value chain that can be found through a hotspot analysis can be a good screening criterion for eco-innovations. However, each Pareto optimal solution will yield different results. Therefore, we choose a compromise value chain that is closest to the utopia point (Figure S1 in the [Supporting Information](#)) in terms of Euclidean distance after normalization of the objectives, described in [section S2](#). This general way of identifying the ideal compromise allows standardization of subsequent analyses to determine key sectors for innovations. The hotspot analysis of the compromise value chain provides the critical sectors of the value chain that contribute the most to the global warming potential and are detrimental to circularity, e.g., plastic losses to the environment. This is done using linear algebra and lifecycle-based allocation methods, which are explained in [section S2](#) and elaborated in Thakker and Bakshi (2021b).<sup>27</sup> Screening of innovations is also performed based on key “sensitive” parameters of the value chain, which can be found using the novel sensitivity-based life-cycle optimization method<sup>30</sup> to find optimal perturbations that lead to win-win solutions. We

implement this prospective approach of identifying potential improvements to supplement hotspot analysis, a retrospective approach.

**Readiness Level (RL) Analysis.** For tie-breaks between innovations in the hotspot or sensitive sectors, we choose innovations to model based on their readiness for adoption.<sup>31</sup> Technology readiness level (TRL) is an extensively studied topic for mechanical and aeronautical innovations. However, it is a critical aspect of ranking eco-innovations since there is an urgent need for deployment of these to meet carbon neutrality and recyclability targets. We consider 10 readiness levels (or stages) for eco-innovations ranging from conceptual and R&D stages (RL = 1 and 2) to Adoption and Maturity (RL = 9 and 10). These derive inspiration from previous studies<sup>32,33</sup> and are elaborated in section S3 of the [Supporting Information](#). Readiness levels (RL), unlike TRLs, are applicable to all innovations, including technological, social, policy, and behavioral domains. Some behavioral innovations like incentives for segregation and reuse will have a readiness level based on the geographical location, type of society (egalitarian, hierarchist, or individualist), and political influence.

**Match Key Sectors and Select Innovations with Highest Readiness Levels.** In recent times several emerging technologies and eco-innovations are being proposed to meet net-zero emissions and circularity targets. Many of them are conceptual, such as new policy or better segregation. Others, which have a quantifiable basis, also rarely contain an anticipatory life-cycle assessment to understand whether they can be adopted in the value-chain network without shifting impacts to other existing processes. The large quantity of these eco-innovations makes it impossible to perform LCA for each alternative and predict synergies between eco-innovations. The proposed methodology can systematically screen from these large lists of conceptual ideas before ranking them, with an implicit assumption that screening based on hotspots and sensitive sectors would identify the eco-innovations expected to have a higher rank. The screening step requires the categorization of the conceptual list of eco-innovations into sectors of the value chain and the readiness level (RL) for adoption. This is typically done by stakeholders and external organizations, such as the “Closing the Circularity Gap” report by Google and AFARA in March 2022.<sup>34</sup> As part of the screening process, the hotspot and sensitive sectors identified in the previous section are matched with the categories (or sector buckets) of conceptual innovations. The innovations in the matched sectors are screened into a smaller list, and readiness level (RL) for adoption is used for breaking ties within the matched sector.

**Data Consolidation.** This step involves performing a preliminary techno-economic analysis of selected innovations to develop “black-box” or simpler linear models representing their steady-state operation. It is expected that, depending on the type of innovation and corresponding value-chain stage, various types of data might already be available. Therefore, this step can either be a relatively straightforward collection of data or a more detailed exercise involving data generation using heuristics, process, or molecular simulations. To model these eco-innovations, typically one must collect information about (a) input raw materials, (b) byproducts, (c) emissions and losses in the process, and (d) energy requirements per unit of output flow to populate the column in the technology and intervention matrices corresponding to the eco-innovation. The input raw materials and energy will be connected to the upstream lifecycle. Similarly, avoided product emissions from generating end-of-life outputs and byproducts are accounted for using displacement. In addition to accounting for these flows, it is also required to collect the prices of circular flows, either from market data or through techno-economic assessments. These prices are needed to calculate the circularity metric ( $\theta$ ). The detailed procedure for updating the lifecycle matrices is described in the final subsection of [Data Consolidation](#) and elaborated in section S4 of the [Supporting Information](#). The next few subsections, however, are meant to demonstrate typical methods that can be used for collecting or generating data for eco-innovations.

**Collection. Literature Survey and Patent Search.** Very often, data required for modeling innovations can be simply obtained from the

academic literature or patents. For instance, technological eco-innovations are usually reported in academic journals if their RL is low and in patents with RL close to commercialization. Innovations screened in the [Screening of Innovations](#) section are predominantly targeted toward chemical recycling and ideated in academic journal articles. To model these, one needs to extract data or generate estimates of transformation yields (from chemical reaction engineering experiments), energy requirements (from enthalpy of reactions), and byproduct profile. For certain catalytic reactions, it might also be necessary to obtain information about makeup catalyst requirements and energy intensity of catalyst production. Energy and reagents required for the transformation can be connected to the upstream life-cycle network to ensure accurate estimation of life-cycle impact of these eco-innovations. In the case where reagents and catalysts are novel and not present in the life-cycle inventory, appropriate assumptions can be made or a separate LCA study can be done to include their impacts within the intervention matrix.

**Estimates from Industrial Reports and Similar Technologies.** For eco-innovations with high RL, it is possible that accurate estimates are concealed for economic advantage over competitors. In such cases, approximate data from industrial reports and analysis of similar innovations may be used to model these eco-innovations. An example for this could be cutting-edge extruders, which can handle larger fractions of recycled content in plastic films. To model such a new technology, one may obtain data from the archives of the company that produces the extruder or from data for conventional extruders with a correction factor.

**Generation. Thumb Rules and Empirical Relations.** In the absolute absence of data and the possibility of simulating the eco-innovation, it is still better to model eco-innovations according to thumb rules and empirical relations rather than ignoring it within the methodology. This principle of utilizing input-output or heuristic data when process design is not possible is aligned with Douglas's hierarchical procedure for process design and synthesis,<sup>35</sup> which uses simple material balance and stoichiometry information for screening among alternatives followed by more detailed information.

**Simulation of Chemical and Mechanical Processes.** Chemical and mechanical process simulation can be used to "generate" data to model eco-innovations. For instance, process simulation software such as Aspen Plus or ChemCAD can be used to simulate either the catalytic chemical recycling process of polyesters or similar plastics or the production of novel feedstocks. Design tools like AutoCAD can be used to model novel extruder designs that, when exported to multiphysics simulation software like ANSYS or Star CCM+, will yield process attributes like maximum permissible recycled content, energy requirements, etc.<sup>36</sup> These attributes can be included in the superstructure network for further evaluation using the steps described in section S4 of the [Supporting Information](#). Another example of mechanical innovations is "Higher sorting efficiency robots" can that use artificial intelligence (AI)-vision analytics.<sup>37</sup>

**Chemistry Knowledge.** Eco-innovations that rely on chemistry are usually in the manufacturing or recycling sectors. For the materials and plastics industries, novel chemistries are being proposed including metabolic pathways utilizing biobased sources and enzymatic reagents.<sup>38</sup> Reaction network flux analysis (RNFA) is a method capable of designing such networks to find optimal reaction pathways for economic and environmental objectives.<sup>39</sup> We have built upon the RNFA framework, developing a multiscale modification (process-to-planet RNFA framework<sup>40</sup>) to include life-cycle and economy flows while finding the implications of adopting a novel chemical-reaction pathway in the existing value chain. This can be used to translate chemistry knowledge to simpler linear programming (LP) models based on molar flux balances for eco-innovations. It is also possible to perform molecular dynamics simulations for systems such as thermal degradation of polymers to obtain product composition, yields, and energy requirements.<sup>41</sup>

**Update Superstructure Network.** The superstructure network needs to be updated to contain the modeled innovations as alternatives. If the innovation is a new technology or a tangible value-chain process, an additional column is added to the super-

structure technology matrix. New rows need to be added if novel products or intermediates are produced, which were not part of the earlier superstructure network. The avoided impact of these products is usually found by means of a separate LCA study and denoted as a negative impact in the column containing the avoided product. Dummy rows and columns need to be added to the technology matrix (A) when the displaced product is already present in the original superstructure, for example, recycled resin or electricity from incineration. Broadly, this process of including novel alternatives within the life-cycle network is undertaken using a system expansion approach, discussed in depth in academic LCA literature<sup>42</sup> and industry-accepted handbooks.<sup>28</sup> The mathematical procedure for appending the superstructure network is provided in [section S4](#). This procedure ensures that the novel technologies, product flows, and input requirements are linked to the upstream life-cycle described by the existing superstructure network, which allows us to consistently compare novel alternatives.

**Innovative Design and Ranking. Optimization to Find New SCE Optimal Value Chains.** After the novel alternatives are appended to the superstructure network, SCE multiobjective optimization is performed on the new superstructure network using the mathematical formulation of the SCE framework, shown in equation S1 of the [Supporting Information](#). This yields a new "innovative" Pareto-front. Notably, introduction of a novel recycling technology or a polymer through eco-innovations leads to a re-evaluation of the choice of bags, collection, and treatment options for the SCE objectives. The integration of novel alternatives with the existing superstructure can possibly lead to synergistic solutions with a selection of different polymers than in conventional value-chain design. Additionally, owing to the fact that novel alternatives are "appended" to the conventional superstructure network, the new Pareto-front is at least as good as the previous one in all the three objective domains. This is because the multiobjective optimization routine would select solutions from the conventional value chain if the innovation underperforms in a particular objective domain.

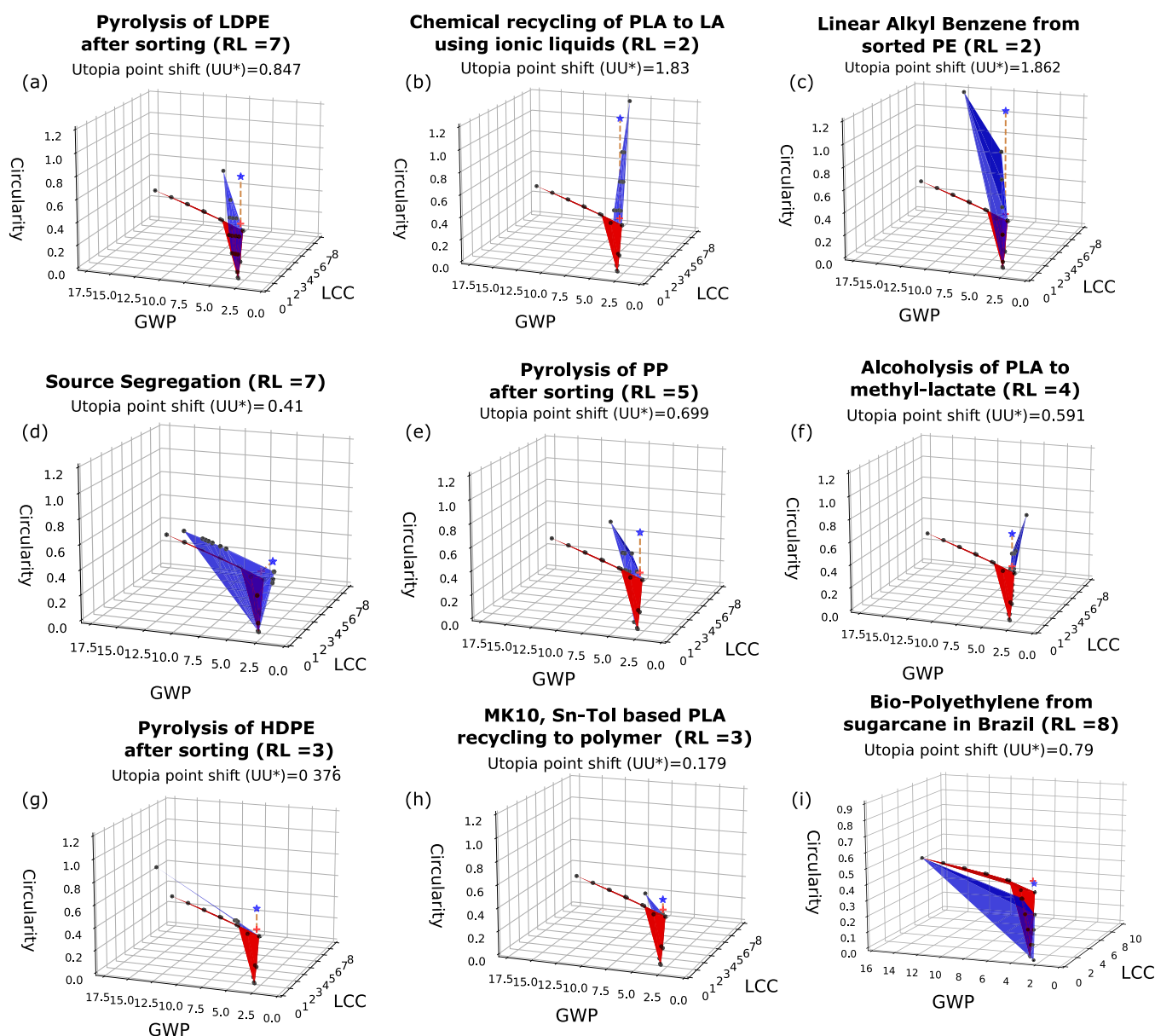
Therefore, it can be concluded that  $\min \text{GWP}_i \leq \min \text{GWP}_o$ ,  $\min \text{LCC}_i \leq \min \text{LCC}_o$ , and  $\max \theta_i \geq \max \theta_o$ , wherein the subscript "i" indicates the new optimal values for the appended superstructure network with innovations and the subscript "o" indicates the optimal values for the conventional or original superstructure network.

**Rank Innovations Based on Shift of Utopia Point and Pareto-Front.** Notably, the coordinates derived from ( $\min \text{LCC}$ ,  $\min \text{GWP}$ ,  $\max \theta$ ) denote the utopia point on the Pareto-front. It can be deduced from the relationship between objective values of the innovative and original value chains that the new utopia point with innovations will be at least as good as the previous utopia point. Therefore, the Euclidean distance between the new and old utopia points can be used as an indicator of the innovation's SCE potential over the conventional value chain. However, the distance needs to be scaled to avoid the effects of different orders of magnitude of each objective. We define the utopia point shift criterion to determine SCE potential of an innovation, as follows.

$$\text{UU}^* = \sqrt{\left[ \frac{\text{GWP}_i - \text{GWP}_o}{\text{GWP}_o} \right]^2 + \left[ \frac{\text{LCC}_i - \text{LCC}_o}{\text{LCC}_o} \right]^2 + \left[ \frac{\theta_i - \theta_o}{\theta_o} \right]^2} \quad (1)$$

Bossle et al. (2016)<sup>31</sup> propose that the market success of an eco-innovation depends on the expected environmental benefit and its future development trajectory. While the utopia point shift captures the benefit in all three domains of SCE, one needs to integrate it with the readiness level of the innovation. Using this philosophy, we define an aggregate metric, which gives a 50% weight to RL value (i.e.,  $\text{RL}/9$ ) and 50% to  $\text{UU}^*/\text{UU}^*_{\max}$  to develop a new ranking criterion (RC). While the expression to aggregate the RL values and shift in utopia point is subjective and can be formulated in many ways based on priority of stakeholders, we have formulated the ranking criteria as follows.





**Figure 3.** Pareto-fronts for nine innovations (a)–(i) (depicted as a blue surface) indicate improvement over original Pareto-front (red surface), with UU\* reported on top of each plot. The axes of each plot represent economic circularity, global warming potential (GWP) and Life-cycle cost of natural resource uptake (LCC). This figure can be used to analyze innovations for preferential direction of win-win, compare utopia shift measure (UU\*), and readiness for adoption.

$$RC = \frac{1}{2} \left[ \frac{RL}{9} \right] + \frac{1}{2} \left[ \frac{UU^*}{UU_{\max}^*} \right] \quad (2)$$

**Termination Criteria.** After the aggregate metric for a particular eco-innovation is computed, it is added to the ranking list based on the magnitude of the metric. The methodology has to terminate when the cumulative ranking list reaches the user-specified length ( $N$ ). If the number of eco-innovations screened is less than  $N$ , the methodology flow returns to the screening step wherein the next eco-innovation is chosen based on the hotspot, sensitivity, and readiness level analysis. Alternatively, the termination criteria can also be more tangible, such as R&D budgets and thresholds on expected emission reductions, set by the stakeholders.

## RESULTS AND DISCUSSION

**Screening.** Since the motivating example for the proposed methodology is to establish an SCE for the grocery bags value

chain, eco-innovations from the packaging domain are screened and ranked to guide future investments. An exhaustive list of conceptual eco-innovations in the packaging domain has been developed by researchers at the Global Kaiteki Center,<sup>43,44</sup> which categorizes eco-innovations based on their (a) readiness level for adoption and (b) targeted value-chain sector.

A major part of the screening step is to identify key sectors in the conventional value-chain network, which are matched with the sector categories in the innovations list to identify the most promising eco-innovations, which are screened for further ranking. Section S2 describes the application of hotspot analysis to the conventional value chain, which illustrates that the highest contributing sectors to GWP and circularity losses are recycling, electricity from coal, waste sorting, and incineration. Similarly, sensitivity-based optimization<sup>30</sup> identi-

**Table 1. Utopia Point Shift and Readiness Level Values for Several Screened Innovations, Ranked Using the Proposed Methodology**

| rank | Pareto front figure | innovation name                                                                       | RL | UU*   | ranking criteria (RC) | % change in |                  |                  |
|------|---------------------|---------------------------------------------------------------------------------------|----|-------|-----------------------|-------------|------------------|------------------|
|      |                     |                                                                                       |    |       |                       | $\theta_u$  | GWP <sub>u</sub> | LCC <sub>u</sub> |
| 1.   | 3a                  | Catalytic pyrolysis of segregated LDPE <sup>49,50</sup>                               | 7  | 0.847 | 0.621                 | 84.6        | 0.0              | 0.0              |
| 2.   | 3b                  | Alkaline hydrolysis of PLA to LA using ionic liquids <sup>47</sup>                    | 2  | 1.830 | 0.611                 | 183.0       | 0.0              | 0.0              |
| 3.   | 3c                  | Linear alkyl benzenes from sorted PE <sup>45</sup>                                    | 2  | 1.826 | 0.610                 | 186.1       | 0.0              | 0.0              |
| 4.   | 3i                  | Biopolyethylene from sugar cane based bioethanol harvested in Brazil <sup>51</sup>    | 7  | 0.797 | 0.603                 | 0.0         | −16.2            | −78.2            |
| 5.   | S4                  | Reduce usage of grocery bags by 30%                                                   | 7  | 0.472 | 0.517                 | 0.0         | −30.0            | −30.0            |
| 6.   | 3d                  | Source segregation by consumers                                                       | 7  | 0.410 | 0.500                 | 18.0        | −37.1            | 0.0              |
| 7.   | 3e                  | Catalytic pyrolysis of segregated PP <sup>49,50</sup>                                 | 5  | 0.699 | 0.469                 | 69.9        | 0.0              | 0.0              |
| 8.   | 3f                  | Alcoholysis of PLA <sup>48</sup>                                                      | 5  | 0.591 | 0.439                 | 58.9        | 0.0              | 0.0              |
| 9.   | 3g                  | Catalytic pyrolysis of segregated HDPE <sup>49,50</sup>                               | 6  | 0.376 | 0.436                 | 37.4        | 0.0              | 0.0              |
| 10.  | 3h                  | Chemical recycling of PLA to polymer using mononitrile clay, Sn/toluene <sup>46</sup> | 3  | 0.179 | 0.216                 | 18.0        | 0.0              | 0.0              |

fies that recycled content and efficiency of recycling are the parameters to which the SCE objectives are most sensitive. These can be perturbed by innovations within the advanced recycling sector. In order to screen from a list of over 100 conceptual eco-innovations,<sup>43,44</sup> we match these key hotspot and sensitive sectors with the sector categories in the compiled list. In case of multiple competing innovations in the same sector, we select the ones with the highest readiness level (RL) for adoption. As an outcome of this exercise, 10 innovations from the plastic packaging industry are screened for inclusion in the superstructure network. Details of this process are elaborated in section S2. The screened innovations along with their sectors and sources of data for inclusion in the model are stated below.

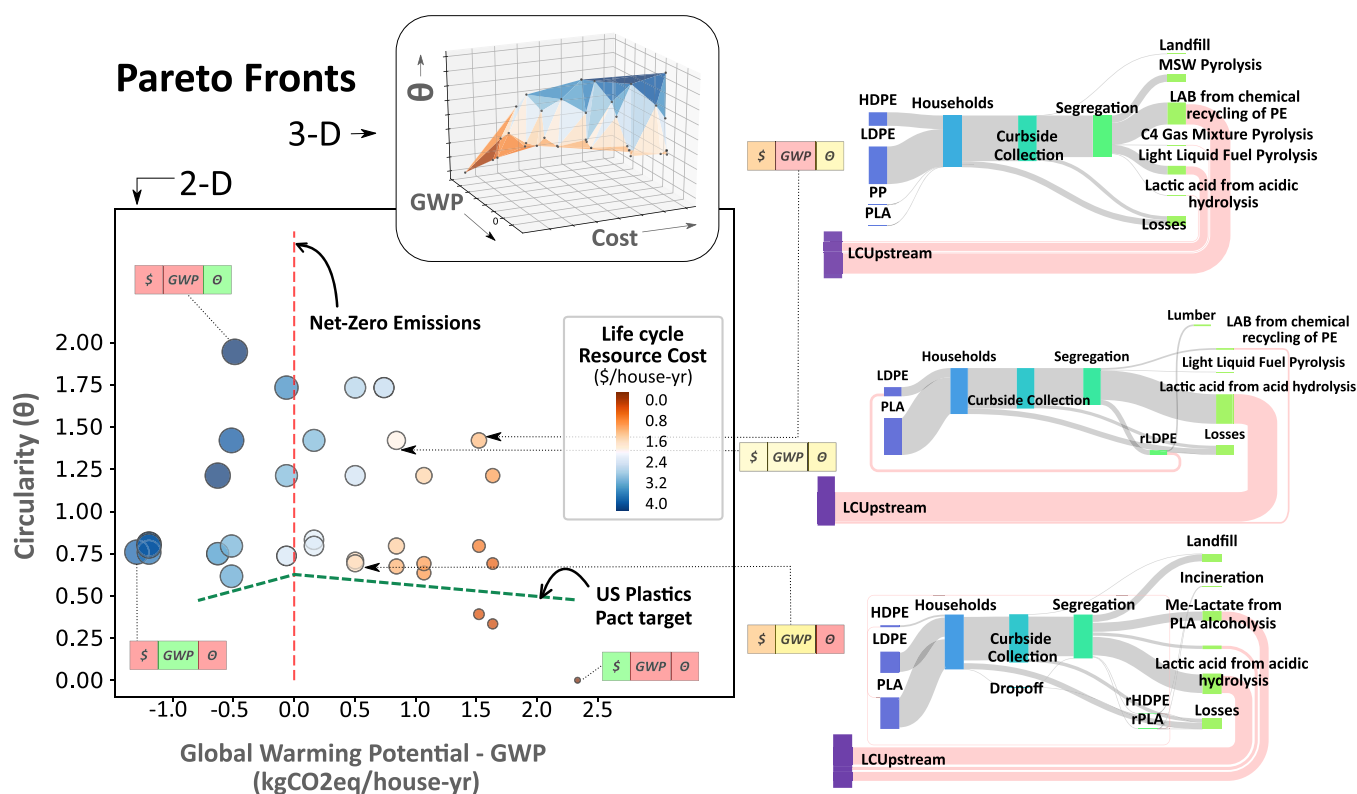
- Recycling and Up-cycling sector
  - (1) Up-cycling of segregated PE to linear alkyl benzenes.<sup>45</sup>
  - (2) Chemical recycling of poly(lactic acid) (PLA) back to polymer pellets using mononitrile clay and tin-based catalysts.<sup>46</sup>
  - (3) Alkaline hydrolysis of PLA to lactic acid in ionic solvents.<sup>47</sup>
  - (4) Alcoholysis of PLA to methyl lactate.<sup>48</sup>
- Household and Segregation sector
  - (1) Source segregation programs.
  - (2) Reduce usage of grocery bags by 30%.
- Energy Recovery sector
  - (1) Catalytic pyrolysis of segregated low-density polyethylene (LDPE) to fuel.<sup>49,50</sup>
  - (2) Catalytic pyrolysis of segregated high-density polyethylene (HDPE) to fuel.<sup>49,50</sup>
  - (3) Catalytic pyrolysis of segregated polypropylene (PP) to fuel.<sup>49,50</sup>
- Upstream Manufacturing
  - (1) Biomass derived polyethylene from sugar cane-based bioethanol.<sup>51</sup>

**Ranking.** After screening 10 innovations from the packaging value chain, data was either collected or generated to model them within the superstructure network, using diverse sets of methods from the Data Consolidation section. The process flow stated in Figure 2 is followed to update the superstructure network with the sequential inclusion of the screened eco-innovations (using the workflow from Figure S3). This is followed by innovative SCE design to develop new

Pareto-fronts for each innovation. These Pareto-fronts are plotted in Figure 3 as blue surfaces against the original Pareto-front representing the currently available technologies (in red). These plots can be used to visualize the trade-offs between SCE objectives and the specific win-win directions in which the eco-innovation leads the value chain. The innovative Pareto-fronts can also be used to determine a favorable innovative value-chain solution, which can be used to infer the ideal percentage of adoption of an eco-innovation in the conventional value chain. Further, the extent of win-win obtained by each of the eco-innovations is measured using the utopia point shift criterion (UU\*). This UU\* measure, in addition to their readiness for adoption (50:50 preference), is used to determine the ranking of these eco-innovations. We terminate the method after ten eco-innovations ( $N = 10$ ) from the large compiled list of over two hundred<sup>43</sup> innovation ideas and concepts are screened and ranked. This termination criterion (after ten eco-innovations) is selected for demonstration purposes; however, users can define termination criteria (number of innovations ranked) based on their investment budgets and resource constraints. The ranking of these ten eco-innovations has been listed in Table 1 and is discussed below.

It can be seen that innovations with higher readiness levels are likely to have a better rank even if they only promise to improve the utopia point marginally. For the grocery-bags example, catalytic pyrolysis (fluid catalytic cracking (FCC) catalyst) of reusable LDPE bags<sup>49</sup> can lead to an overall improvement of SCE objectives while also being in the commercialization stage. It is hindered because of segregation constraints and corresponding energy needs, as the pyrolysis fixed-bed reactor requires a pure feed stream. Novel technologies for up-cycling polyethylene and recycling poly(lactic acid) to pure-form lactic acid have a lower readiness level but promise to greatly improve SCE objectives. This finding can be used to recommend relevant industries such as waste management to invest in such technologies for long-term returns. However, a more detailed cost-benefit analysis will be required to evaluate the return on investment including capital and fixed costs. Notably, source segregation is a social innovation that can also have a significant impact on utopia-point shift (win-win), but it can have a limited increase in circularity if not coupled with other recycling techniques for end-of-life. Realistically, its readiness for adoption is hindered by human behavior, the logistics of installing separate bins, and arranging for separate transport vehicles. Another behavioral





**Figure 4.** Pareto-front of the future, found by performing SCE design on a superstructure network with nine eco-innovations (all but reduction in usage). The Pareto-front is projected on a 2-D axis with the third objective (LCC) depicted through the size and color of the scatter points. The Sankey diagrams denote the material flows corresponding to the compromise value chains with unique eco-innovation combinations. Solutions for single-objective optima are shown in Figure S4. The annotations with three columns indicate the relative performance of the value chain in each of the three objectives; green background indicates the best value for the objective, and the color scale from yellow to red indicates the incremental worsening of the corresponding objective.

innovation considered in this study is reduction in usage of grocery bags all together and switching to personal carry bags with considerably long lifetimes ( $\geq 4$  years), which are used also for other utilities. A 30% reduction in usage results in a significant utopia point shift, and this “reduce”-based innovation is ranked highly (5) among other technological and societal innovations, reinforcing the “reduce, reuse, and recycle” model, which promotes reduction before other circularity-related interventions. While this behavioral innovation is described in section S5 of the Supporting Information, it has been excluded from further analyses since it is difficult to evaluate the cost and impact of introducing this innovation. Additional information about spatiotemporal variation in perception toward environmental issues is also needed to estimate an accurate RL value. The additional emissions for these activities have been approximated in the interventions matrix corresponding to this innovation. Similar to these top four candidates, inferences can be made for the other eco-innovations using the utopia-point shift criterion. The developed methodology (Figure 2) is powerful not only because it can quantify the actual benefits that can be obtained from the life-cycle network but also because it can reduce the computational load of large-scale data consolidation and superstructure optimization for over 100 eco-innovations to a subset of most-promising screened innovations.

After determining the eco-innovation ranking, the stakeholders might want to find an optimal combination of these eco-innovations in a future value chain, when all of these innovations become adoptable. We propose to facilitate this by

performing innovative SCE design while considering all of these eco-innovations simultaneously in the superstructure network. This yields a new Pareto-front for the future, depicted in Figure 4. Most interestingly, it can be seen that the future Pareto-front crosses the net-zero emissions and US plastics pact barriers providing reassurances that the screened eco-innovations can help us meet climate change and circularity pledges such as the Paris accord. Notably, none of the screened eco-innovations are independently able to be net-zero emissions, but their synergies and combinations permit zero and even net-negative emissions from Pareto-optimal value chains. Particularly, source segregation coupled with chemical recycling techniques lead to a substantial reduction in GWP. It is also worthwhile to note that solutions above the green dotted line (most points on the Pareto front) have a recycled and/or biobased content higher than 30% as per the targets set by the US Plastics Pact for 2025. Despite the low GWP and higher circularity in future value chains, there still exists a trade-off between the three objectives. This is evident from Figure 4 in which the future Pareto-front is stretched out in all three directions as compared to individual Pareto-fronts in Figure S1. This is because many intermediate win-win-lose (or compromise) solutions can be obtained from combinations of various eco-innovations and mature technologies in different parts of the value chain. The stakeholder can now pick a compromise solution from the new Pareto-optimal set and determine the ideal combination for future investment. Figure 4 shows three such compromise solutions on the future Pareto-front with two unique eco-innovation combinations, depicted

as Sankey diagrams. These Sankey diagrams depict the material flows within the value chain corresponding to the Pareto-optimal solutions. The products from up-cycling or down-cycling waste are also directed to the Life Cycle Upstream (LCUpstream) in Figure 4. The border solutions for optimizing each of the objectives (described in section S5) are often not desired because they usually lead to extremely bad solutions for the other objectives. For this study, we focus on decisions of the carrier bags value chain and omit innovations from the upstream lifecycle (e.g., power generation, transport, supply chain) and downstream alternatives such as carbon capture and use, to limit the scope of the paper and to focus mainly on the methodology.

While one of the depicted compromise solutions (bottom right of Figure 4) has a reduced global warming potential at the cost of circularity, the other (top right of Figure 4) improves circularity while resulting in higher global warming potential. The former solution consists of using LDPE and biobased poly(lactic acid) to make bags, followed by segregation and end-of-life treatment through pyrolysis and alkaline hydrolysis, respectively. The higher economic circularity compromise solution, on the other hand, promotes using polyethylene bags and up-cycling to linear alkyl benzenes. The right-center Sankey diagram corresponds to the compromise solution closest to the utopia point in terms of Euclidian distance in the normalized objective space. In the absence of a stakeholder preference, this solution can be assumed to be a reliable choice from the Pareto optimal set. It corresponds to a value-chain solution with high composition of PLA bags being source-segregated and being hydrolyzed back to lactic acid. It is worthwhile to note that, given the stakeholder's relative preference for sustainability versus circularity, the methodology can provide a Pareto-optimal strategy for investing in future value chains.

## CONCLUSIONS

This work provides a methodological framework to screen and rank conceptual eco-innovations being proposed for sustainability and circularity, using a quantifiable basis. This eco-innovation ranking methodology allows corporations and governing bodies to systematically screen and select alternatives, in order to meet their future targets of reducing their global warming potential and increasing circularity, while incurring a reasonable cost. Since the underlying computational structure is based on life-cycle assessment and design, ranking of eco-innovations is done based on a holistic system boundary with more confidence that environmental impact does not shift to other parts of the innovative value chain. Multiobjective optimization makes it possible to calculate the trade-offs between environmental impact, resource use, and circularity while adopting eco-innovations. Selection of a solution on an innovative Pareto-front will allow the user to determine the ideal extent of adoption of an eco-innovation in the conventional value chain. The ranking criterion within the proposed method focuses on the win-win potential of eco-innovations with respect to the objectives, thereby allowing multicriteria decision making for investment in the innovations. Once the methodology flow is terminated and the specified number of ranked eco-innovations are obtained, future Pareto-fronts can be developed by simultaneously including all the screened ( $N$ ) eco-innovations in the superstructure network, thereby providing the user an ideal combination of eco-innovations to invest in, for highest returns

in the future. The screening step in the methodology also addresses practical limitations that arise when very many eco-innovations need to be evaluated and modeling efforts and data sources are limited. This step utilizes hotspot and sensitivity analyses to determine which eco-innovations are most likely to bring about the highest improvement in each objective. In turn, this reduces the computational burden on the data consolidation step. In summary, the methodology proposed in this work will be useful to policy makers, corporate organizations, and funding agencies to determine the best eco-innovation to invest in, for achieving win-win solutions. The ranking along with readiness level values would also aid in planning sustainability transitions toward net-zero economies of the future.

Application of the proposed methodology is demonstrated for ranking eco-innovations in the plastic packaging industry, which can be introduced in a grocery bag value chain. The win-win ranking criteria developed using RL values and UU\* in the Methods section is utilized to screen and rank nine conceptual innovations from an exhaustive list of over 200 eco-innovations. A Pareto-front for the future is generated to identify the relative prevalence of each eco-innovation in a compromise value chain chosen by the stakeholder. This new Pareto-front can also be used to gauge how close the stakeholder, including corporations or governments, can get to net-zero emissions and circularity targets through the screened eco-innovations. For the grocery bags example, value chains adhering to the US plastics pact and net-zero climate change pledges are possible through synergies of source-segregation, biobased polyethylene production, and chemical recycling to fuel feedstock. This provides an incentive for further research in the chosen eco-innovations and discovers synergies for meeting environmental pledges. Since the innovations list in this case study only pertains to the packaging industry, it mainly selects innovations from the chemical industry that increase the circularity of the system, such as end-of-life treatment of waste using pyrolysis or chemical recycling. However, if a corporation intends to use this framework for implementing their decarbonization and net-zero emissions strategies, the innovations list would also have to include technologies such as carbon capture and storage, renewable feedstock and energy, green and blue hydrogen, etc.

With growing interest and research in LCA of these novel technologies, the proposed method can rank these technologies by appending their life-cycle impact assessment results to the superstructure, as described in the Methods section. The introduction of these decarbonization alternatives will further highlight the utility of the multiobjective optimization-based ranking method to systematically allocate future investment between recycling-centric and renewable-centric options. While the proposed methodology can efficiently screen and rank eco-innovations for preliminary evaluation by investing companies, it is essential to consider absolute sustainability, nature's carrying capacity of ecosystem services (such as carbon sequestration, air- and water-quality regulation, etc.), and natural resource availability, before adopting these innovations. Integrating these attributes as environmental objectives correctly<sup>7</sup> requires spatially explicit data and inclusion of the Techo-Ecological synergy<sup>22,23</sup> framework, which is part of ongoing work. The other shortcoming of this methodological framework is that the results heavily depend on life-cycle inventory data and the quality of consolidated

data. It is, therefore, essential to include effects of uncertainty associated with LCA and the data collection/generation steps, through Monte Carlo simulations and sensitivity analyses. For large-scale substitution of pre-existing products by down- and up-cycled material through eco-innovations, it will also be critical to include consequential aspects of LCA to the design methodology in future work. These aspects will introduce marginal effects, market elasticity, and economies of scale through previously developed multiscale models,<sup>40,52</sup> thereby allowing the UU\* metric to also prioritize investments based on production scalability. Future work will also focus on development of roadmaps for eco-innovations with a goal of facilitating a transition to a net-zero economy. The innovation Pareto-fronts developed as an outcome of this work will provide a basis for the roadmap planning problem. In addition, this effort will require consideration of evolution of innovation RL values over time and future scenarios of background emissions based on shared socioeconomic pathways.

## ■ ASSOCIATED CONTENT

### SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acssuschemeng.2c05732>.

Description of the Sustainable Circular Economy (SCE) framework; SCE solutions for the current grocery bags' value chain; Readiness level scale; Steps for updating superstructure network; Border solutions of the Pareto-front in Figure 4; Effect of reduction in usage ; Alternative termination criteria and Data sources for modeling innovations. The superstructure network data for the conventional value chain is available from Thakker and Bakshi 2021b.<sup>27</sup> The information for modeling innovations is made available along with the code for implementation in the form of a supporting zenodo data set<sup>53</sup> (PDF)

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### Notes

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