

MULTI-PERIOD OPTIMIZATION OF MULTI-AGENT CIRCULAR ECONOMY NETWORKS: APPLICATION TO SINGLE-USE PET PLASTICS AND POLYESTER TEXTILES

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Abstract

Agents in supply chains (SCs) must take different initiatives over time in order to enable the transition to a circular economy (CE). However, different agents often have competing objectives, which may not align with each other and may result in undesirable effects on the circularity of the overall supply chain, including burden-shifting between agents. Furthermore, the use of frameworks such as Circulytics [1] to assess circularity at the agent level may also result in burden-shifting.

Although SC and superstructure optimization models have been widely employed to find optimal circular network designs [2, 3, 4, 5, 6, 7], most models rely on centralized optimization of network-level objectives rather than considering the objectives of different agents. Understanding how well agent- and network-level objectives align and whether optimal CE network designs benefit some agents at the expense of others would enable the development of more holistic agent-level circularity indicators and help stakeholders prioritize efforts to improve circularity. In addition, with the exception of [8], most CE frameworks only apply to a specific case study, limiting their generalizability to different case studies or systems in which material from one application is used for another.

Previously, we developed a generic framework for dynamic modeling of CE networks with multiple agents and used it to study the value chain for single-use polyethylene terephthalate (PET) plastic packaging in the US [9]. Here, we formulate this framework as an optimization model and consider an extended version of the PET value chain that includes polyester textiles and chemical recycling. Life cycle assessment (LCA) is combined with the planetary boundaries framework [10, 11, 12] to assess environmental impact. We use multi-objective optimization to find trade-off solutions that balance network-level circularity, environmental impact, and different agents’ net present values and Circulytics scores over a 15-year time horizon.

Our findings agree with previous work that there are trade-offs between circularity and sustainability. For the PET case study, combining glycolysis and mechanical recycling of packaging with “downcycling” of textiles to lower-quality fiber applications outside the PET value chain minimizes environmental impact, while “upcycling” of textiles into packaging via methanolysis and mechanical recycling of packaging maximizes circularity. However, all Pareto-optimal trade-off solutions outperform the baseline linear economy. Although improved network-level circularity generally leads to increased agent-level circularity, the reverse is not always the case. Furthermore, improvements in one agent’s circularity often come at the expense of other agents’ circularity or environmental impact. Therefore, there is a need for improved agent-level circularity indicators that avoid burden-shifting.

Introduction and Motivation

The transition to a Circular Economy (CE) requires the concerted effort of many agents across supply chains (SCs) to take different initiatives over time. These initiatives often require significant up-front investments or organizational changes, and their benefits may depend on the behavior of other agents. As a result, analytical frameworks have been proposed to assess the circularity of the proposed initiatives with the aim of predicting which ones will be more successful. These frameworks aim to assess circularity at the agent, product, and network levels using various indicators. Examples of frameworks for assessing agent-level circularity include MICRON [13], Circulytics [1], and the Circular Transition Indicators (CTI) [14], which are frequently used in corporate sustainability reporting. The Material Circularity Indicator (MCI) [15] and “Degree of Circularity” [8] are examples of product-level and network-level indicators. However, one level of

circularity may not translate to another; in particular, increasing circularity at the agent level may not result in an increase of circularity at the network level. For example, if a manufacturer increases its circularity by using more recycled material, demand for recycled material may also increase, raising its price. In response, waste collection agencies may pay consumers more to collect their waste, causing consumers to use products for less time before discarding them, thereby increasing consumption levels. This increase in consumption levels may actually result in more resources extracted from the Earth, which decreases overall circularity.

In our previous work [9], we presented a generic, modular framework for dynamic modeling of multi-agent CE networks that included five agent types: manufacturer, consumer, material recovery facility (MRF), recycling facility, and the Earth. The framework accounted for consumer reuse and recycling behavior while estimating required capacity expansion of the involved firms as well as material quality loss due to recycling. We combined the models for the five agents to form a model for a prototypical CE network. We used this model to study a simplified version of the SC for single-use polyethylene terephthalate (PET) plastic packaging in the US.

Here, we extend that work by formulating the previously developed framework as an optimization model using a multi-period state-task network (STN) formulation [16] in which the states are stock nodes, or inventories of material, and the tasks are technology nodes, or processes that convert material from one form to another. This formulation can be used to define a superstructure representation for an arbitrary multi-agent circular SC network. We use multi-objective optimization to assess the trade-offs between network-level and agent-level circularity, economic, and environmental objectives for an extended version of the previously considered PET supply chain.

Review of Related Work

SC optimization models in the context of CE include the work by Wang and Maravelias, who developed a series of Mixed Integer Linear Programming (MILP) formulations for a facility location problem involving a generic mixed plastic waste management system that includes the effects of composition and sorting on recyclability as well as capacity constraints and transportation costs [2]. The authors used this model to optimize a combined economic and environmental objective.

Chaudhari et al. combined life cycle assessment (LCA) and material flow analysis to develop a systems analysis framework and used it to formulate a linear program to minimize the global warming potential (GWP) of a closed-loop supply chain for polyethylene terephthalate (PET) bottles [17]. In a follow-up article [3], Chaudhari et al. extended this model to include facility location decisions, additional recycling pathways, additional types of plastics, and additional types of plastic packaging manufacturing processes. They used an MILP formulation to minimize the GWP and cumulative energy demand (CED) of the PET and polyolefin (PO) packaging SCs in the US, finding that the optimal circular design achieves a lower GWP and CED relative to the baseline linear economy. This model is extended further in [18] to use multi-objective optimization to determine the optimal selection of recycling technologies that balance trade-offs between environmental impact and socio-economic objectives for the “cradle-to-cradle” PET packaging SC in the US, finding that there is no unique selection of technologies that results in optimal outcomes for all objectives, and optimal decisions depend on stakeholder preferences. However, the study does not consider polyester textiles, a significant part of the PET value chain and a possible source of recycled feedstock, and assumes that 100% of the waste packaging is recycled. However, only a fraction of the waste PET packaging is recycled in the US [19]. Hernández et al. use multi-objective superstructure optimization to balance trade-offs between economic and environmental objectives for the low-density-polyethylene (LDPE) recycling SC [20]. However, these models assume that the network operates at steady state and do not consider the time dimension. As a result, they cannot consider time-dependent effects such as the delay of end-of-life product flows due to consumer reuse or “downcycling” of end-of-life products to other applications with different lifetimes. In addition, static models cannot consider the path-dependency of the transition from a linear to a circular economy over time, which may be hindered by “lock-in” on a suboptimal state [21].

Optimization models that incorporate the time dimension include the work by Alumur et al., who proposed a generic, multi-period reverse logistics supply chain design model that considers multiple products with multiple components [22]. The model is formulated as an MILP and used to optimize the profit of the circular supply chain for washing machines and tumble dryers in Germany. Badejo et al. proposed a multi-period MILP model for determining the optimal technologies, locations, installation timelines, and

operational decisions for plastic waste management SCs and use it to optimize the circularity, profit, and global warming potential (GWP) of the LDPE SC in the US from the present day to 2050. Similarly to [18], they find that different recycling technologies are selected for each objective, highlighting the difficulty of simultaneously meeting both the circularity and the decarbonization goals. However, they do not use multi-objective optimization to find trade-off solutions or consider environmental impacts beyond GWP.

Since most optimization models only consider network-level objectives without considering the objectives of individual agents, the solutions obtained may benefit some agents at the expense of others. As a result, some firms may choose not to participate, making such solutions unlikely to be achieved in practice. In addition, although some models consider agent-level economic objectives, those that do have limited generalizability to different case studies or systems, in which material from one application is used for another. Furthermore, few studies consider agent-level circularity objectives. As a result, there is a lack of understanding of how well agent-level circularity translates to network-level circularity and environmental sustainability. Although [5] uses multi-objective optimization to balance trade-offs between agent-level economic and circularity objectives using MICRON, they only consider a single agent, a packaging manufacturer who takes responsibility for recycling post-consumer waste, and do not consider network-level circularity as an objective. Therefore, generic optimization frameworks that consider stakeholder objectives would help prioritize efforts to maximize circularity while minimizing burden-shifting among agents and promoting win-win solutions. If improvements in circularity indicators lead to burden-shifting of environmental impacts to other agents, it means that they fail to measure true circularity, diminishing their value. Furthermore, it could result in undesirable effects on broader sustainability goals if used in corporate sustainability reporting, becoming yet another example of “greenwashing”. An example of a win-win solution where multiple stakeholders benefit from circularity initiatives is industrial symbiosis, where one firm sells its waste material to another firm that finds a valuable use for it. For example, whey protein is a by-product of the cheesemaking process and in the past was dumped into rivers, harming wildlife health. Nowadays, whey protein is sold to manufacturers of protein powder instead, which has helped reduce pollution [23].

Technology Approach

The generic model for an agent is shown in **Figure 1** below. Each agent exchanges material with other agents, performs composition transformations on the material via one or more technology nodes, and stores material in the form of one or more stock nodes. Let T be the set of time periods t , A be the set of agents a , I be the set of material components i , J be the set of technology nodes j , $K \subset A \times I$ be the set of stock nodes $k = (a, i)$, each of which represents the inventory of component i held by agent a . To reduce the problem size, we divide the set of stock nodes into material stock nodes (K_M), which can accumulate material as inventory, and non-material stock nodes (K_{NM}), which cannot.

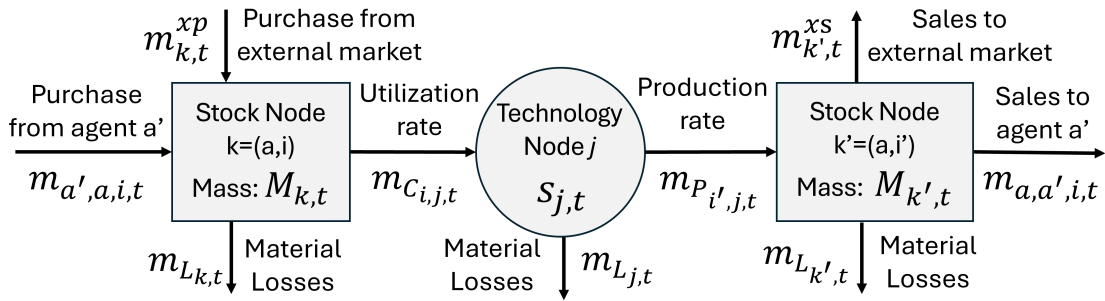


Figure 1: General structure of agent a . Here $m_{C_{i,j,t}}$ and $m_{P_{i',j,t}}$ are the consumption and production rates of component i by technology node j at time t , $m_{a',a,i,t}$ is the rate of purchase of component i by agent a from agent a' , $m_{L_{k,t}}$ is the rate at which material is discarded from stock node k , and $m_{k,t}^{xp}$ and $m_{k,t}^{xs}$ are the purchase and sales rates between stock node k and the external market at time t .

The material balance on each material stock node k is given by Equation (1) as the sum of the inlet flows minus the sum of the outlet flows. Here $M_{a,i}$ (or equivalently, M_k) is the mass of inventory held in material

stock node $k = (a, i)$ at time t and other variables are described in Figure 1. $J_a \subset J$ and $K_a \subset K$ are the sets of technology nodes and stock nodes belonging to agent a . The material balance on each non-material stock node is similar but with the right-hand side set equal to zero since any material entering the stock node must be used in the same time period.

$$\frac{dM_{k,t}}{dt} = \sum_{j \in J_a} (m_{P_{i,j,t}} - m_{C_{i,j,t}}) + \sum_{\substack{a' \in A \\ a' \neq a}} (m_{a',a,i,t} - m_{a,a',i,t}) - m_{L_{k,t}} + m_{k,t}^{xp} - m_{k,t}^{xs} \quad \forall k \in K_M \quad \forall t \in T \quad (1)$$

The material balance on each technology node $j \in J$ is given by Equation (2), where $s_{j,t}$ is the scaling factor, or total material flow rate through technology node j at time t , $m_{L_{j,t}}$ is the rate at which material is lost as processing waste, and $I^{in}(j)$ and $I^{out}(j)$ are the sets of components consumed and produced by technology node j . The production ($m_{P_{i,j,t}}$) and consumption ($m_{C_{i,j,t}}$) rates of each component are given by Equation (3) and Equation (4), respectively. Here, $\gamma_{i,j}$ is a normalized conversion factor given by the technology matrix, which describes the component transformations associated with each technology [24], which is negative (or positive) if component i is consumed (or generated) by technology node j and zero otherwise. Since $\gamma_{i,j}$ is normalized by the total flow through a technology node, it lies between -1 and 1. Equation (5) limits the scaling factor of a subset $J_{cap} \subset J$ of technology nodes by some maximum processing capacity ($Capacity_{j,t}$), which may be expanded over time. Furthermore, the scaling factor must exceed some minimum fraction ($MinUtil_j$) of the total installed capacity. If E is the set of environmental impacts e , we assume that technology node j contributes to impact e at a rate of $Imp_{e,j,t}$ at time t , which is given by Equation (6). We assume impacts are proportional to the scaling factor by the impact factor $g_{e,j}$, which is obtained from the ecoinvent 3.10.1 LCA database using the TRACI v2.1 impact assessment method [25, 26].

$$s_{j,t} = \sum_{i \in I^{in}(j)} m_{C_{i,j,t}} = m_{L_{j,t}} + \sum_{i \in I^{out}(j)} m_{P_{i,j,t}} \quad \forall j \in J \quad \forall t \in T \quad (2)$$

$$m_{P_{i,j,t}} = \gamma_{i,j} \cdot s_{j,t} \quad \forall i \in I^{out}(j) \quad \forall j \in J \quad \forall t \in T \quad (3) \quad m_{C_{i,j,t}} = -\gamma_{i,j} \cdot s_{j,t} \quad \forall i \in I^{in}(j) \quad \forall j \in J \quad \forall t \in T \quad (4)$$

$$MinUtil_j \cdot Capacity_{j,t} \leq s_{j,t} \leq Capacity_{j,t} \quad \forall j \in J_{cap} \quad \forall t \in T \quad (5)$$

$$Imp_{e,j,t} = g_{e,j} \cdot s_{j,t} \quad \forall e \in E \quad \forall j \in J \quad \forall t \in T \quad (6)$$

Design objectives

Network-level circularity

Since circular flows such as recirculated products and recycled materials are often difficult to measure but lower the amount of linear flow that enters and exits the system, we use linear flow as a proxy for circularity, with increased linear flow per unit of product meaning lower circularity at the same scale. The Mean Linear Flow is given by Equation (7) as the time average of the total linear flow, which is given by Equation (8) and includes virgin raw material production, purchases from the external market, sales to the external market with a time delay associated with the product lifetime, disposed waste from stock nodes, and material losses from technology nodes. Here, P is the set of products p and J_V is the set of life-cycle upstream technology nodes that represent the cradle-to-gate impacts of virgin feedstock production [8]. To account for the amount of raw material required to produce any initial in-use stocks of products p , we include a term for the initial mass of in-use stocks normalized by the manufacturing yield (η_{MF_p}).

$$\min \quad \text{Mean Linear Flow} = \frac{1}{|T|} \left(\sum_{t \in T} \text{LinearFlow}_t + \sum_{p \in P} \frac{M_{C,p,0}}{\eta_{MF_p}} \right) \quad (7)$$

$$\text{LinearFlow}_t = \sum_{j \in J_V} \sum_{i \in I^{out}(j)} m_{P_{i,j,t}} + \sum_{k \in K} m_{k,t}^{xp} + \sum_{k \in K} m_{k,t-\lambda_k}^{xs} + \sum_{k \in K} m_{L_{k,t}} + \sum_{j \in J} m_{L_{j,t}} \quad \forall t \in T \quad (8)$$

Agent-level circularity

The circularity of a subset of agents, including manufacturers, MRFs, and recyclers ($a \in A_{circ}$) is measured using Circulytics [1]. The Circulytics score of agent a at time t ($Circ_{a,t}$) is given by Equation (9) as the weighted average of the theme scores ($scr_{a,h,t}^{theme}$), with each theme $h \in TM_a$ given a weight of w_h^{theme} . Here TM_a be the set of themes that apply to agent a . We consider the themes of Products and Materials, Water, and Energy. The score for each theme h is given by Equation (10) as the weighted sum of the scores ($scr_{a,n,t}^{indic}$) for each indicator $n \in N_h$ in theme h . Each indicator n is weighted by $w_{a,n,t}^{indic}$. Each theme score is normalized by the sum of the indicator weights so that the effective weights sum to one.

$$Circ_{a,t} = \sum_{h \in TM_a} \left(w_h^{theme} \cdot scr_{a,h,t}^{theme} \right) \quad \forall a \in A_{circ} \quad \forall t \in T \quad (9)$$

$$scr_{a,h,t}^{theme} = \sum_{n \in N_{h,a}} w_{a,n,t}^{indic} \cdot scr_{a,n,t}^{indic} \quad \forall h \in TM_a \quad \forall a \in A_{circ} \quad \forall t \in T \quad (10)$$

Holistic environmental impact assessment: Earth system impact metric (ESIM)

We use the planetary boundaries (PBs) framework [10, 11] to quantify absolute environmental sustainability (AES), or the extent to which the environmental impacts of a CE network exceed the restorative capacity of the Earth [27]. PBs are threshold values for “control variables”, or metrics describing human impacts on different “Earth-system processes” (ESPs) beyond which there is an increasing risk of destabilization. Let B denote the set of ESPs. The “safe operating space” (SOS) for each ESP $b \in B$ is defined as the difference between the value of its control variable at the PB and the pre-industrial level. To enable the use of the PBs framework to assess the AES of a SC network, a Share of the Safe Operating Space (SoSOS) given by Equation (11) is allocated to the network for each ESP based on the market size of each product relative to global gross domestic product (GDP_{global}). Direct impacts on ESP b are denoted by $d_{b,t}$ and are given by Equation (12) as the product of each environmental impact flow ($Imp_{e,j,t}$) and a characterization factor $CF_{e,b}$ relating flow e to ESP b , normalized by the SoSOS. The amplified impact of the network on ESP b after accounting for feedback interactions is denoted by $\Delta x_{b,t}$ and given by Equation (13). Here $a_{b,b'}$ is the interaction strength describing the impact of the control variable for process b' on process b and is given by the amplification matrix obtained from Lade et al. [28].

$$SoSOS_b = SOS_b \times \sum_{p \in P} \frac{MarketSize_p}{GDP_{global}} \quad \forall b \in B \quad (11) \quad d_{b,t} = \frac{\sum_{e \in E} CF_{e,b} \sum_{j \in J} Imp_{e,j,t}}{SoSOS_b} \quad \forall b \in B \quad \forall t \in T \quad (12)$$

The Earth system impact metric (ESIM) proposed by Lade et al. [29] is an aggregated measure of impact on different Earth-system processes. It is defined by Equation (14) as the weighted sum of the amplified impacts of the network on each ESP, with weights given by the current values of the global-scale control variables normalized by their SOS and clipped to be between zero and one ($\text{clip}(x_b^{global})$).

$$\Delta x_{b,t} = \sum_{b' \in B} a_{b,b'} d_{b',t} \quad \forall b \in B \quad \forall t \in T \quad (13) \quad ESIM_t = \sum_{b \in B} \text{clip}(x_b^{global}) \cdot \Delta x_{b,t} \quad \forall t \in T \quad (14)$$

We aggregate all of the agents and ESPs in the ESIM to obtain a single metric that quantifies the environmental impact of a SC network. Considering each of the ESPs and agents separately would increase the dimensionality of the Pareto front and make the results harder to interpret. It is also not straightforward to allocate an SoSOS to an individual agent, especially since different agents often have inherently different levels of impact. For example, manufacturing usually has a much larger impact than sorting at an MRF.

Economic objective: Net Present Value (NPV)

Economic objectives include the net present value (NPV) of each agent a , which is given by Equation (15) as the discounted sum of the net profits ($Profit_{a,t}$) in each time period, which are given by Equation (16). Here ρ is the discount rate, c_D is the disposal cost, $\pi_{a,i}$ is the selling price of component i , $Inst_{j,t}$ is the

number of plants of technology node j installed at time t , and $CAPEX_j$ and $OPEX_j$ are the capital and operating costs of technology node j .

$$NPV_a = \sum_{t=0}^{t_f} \left(\frac{1}{(1+\rho)^t} \text{Profit}_{a,t} \right) - \sum_{j \in J_a} (CAPEX_j \cdot \text{Capacity}_{j,t=0}) \quad (15)$$

$$\text{Profit}_{a,t} = \sum_{i \in I} \left(\pi_i \cdot \left(-m_{k,t}^{xp} + m_{k,t}^{xs} + \sum_{a' \in A} (m_{a,a',i,t} - m_{a',a,i,t}) \right) \right) - \sum_{j \in J_a} (CAPEX_j \cdot \text{Inst}_{j,t} + OPEX_j \cdot s_{j,t}) - c_D \left(\sum_{k \in K_a} m_{L_{k,t}} + \sum_{j \in J_a} m_{L_{j,t}} \right) \quad (16)$$

Case study: PET supply chain

The framework is applied to study the value chain for PET plastic in the US. The superstructure representation of the agents and technologies considered is shown in **Figure 2**. We consider three products: single-use bottles, reusable thermoform packaging, and polyester textiles. The quality of PET resin is measured by the intrinsic viscosity (IV), which we assume must be above a certain threshold for each product [30]. Since we assume the mechanical recycling process reduces IV by a constant factor [31], after a certain number of cycles, material must be blended with virgin PET to meet minimum quality requirements. Collection rates were initialized to their current values in the US: 26.6%, 9%, and 14.7% for bottles, thermoforms, and textiles, respectively [19, 32, 33]. We assume that collection rates can change by at most 5% per year. However, higher collection rates would likely increase circularity levels. To establish a baseline, representing the current “linear economy” in which most waste is landfilled, the model was run with collection rates, capacities, and post-consumer recycled contents fixed at their current levels. The model was implemented in Pyomo as a quadratically constrained program (QCP) and solved using IPOPT [34, 35, 36]. Differential equations were discretized using the implicit Euler method via Pyomo.DAE [37]. The ϵ -constraint method was used to obtain Pareto-optimal trade-off solutions that balance different objectives [38].

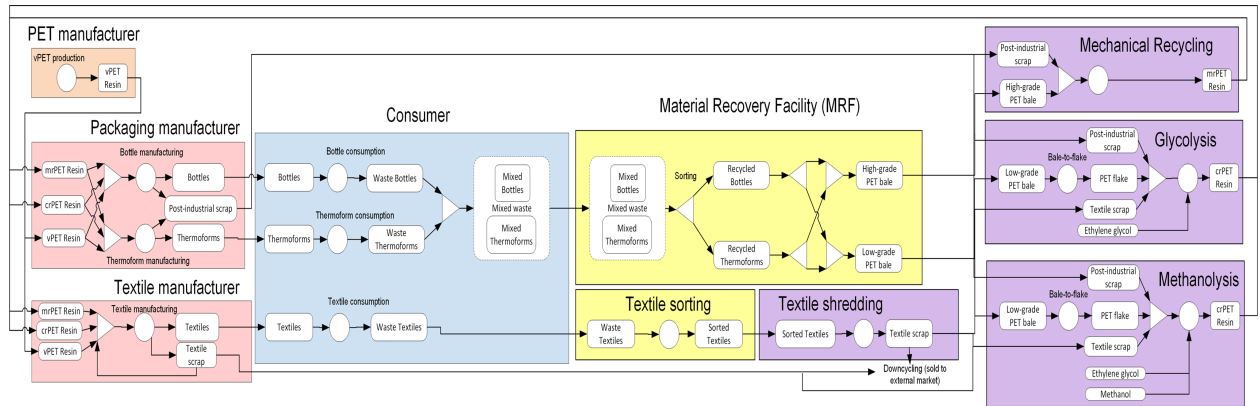


Figure 2: Superstructure of PET CE network with virgin PET (vPET) manufacturer (orange), manufacturers (red), consumer (blue), MRFs (yellow), and recyclers (purple). Blocks represent agents ($a \in A$), rounded rectangles represent stock nodes ($k \in K$), circles represent technology nodes ($j \in J$), and triangles represent mixing and splitting operations.

Discussion

The solutions that minimize the Mean Linear Flow and Mean ESIM and the Pareto front of trade-off solutions balancing the objectives are shown in **Figure 3**. Solution (c) minimizes the Mean ESIM by combining glycolysis and mechanical recycling of packaging with “downcycling” of textiles to lower-quality fiber applications outside the PET value chain (e.g., insulation and filling material), which we assume have a lifetime

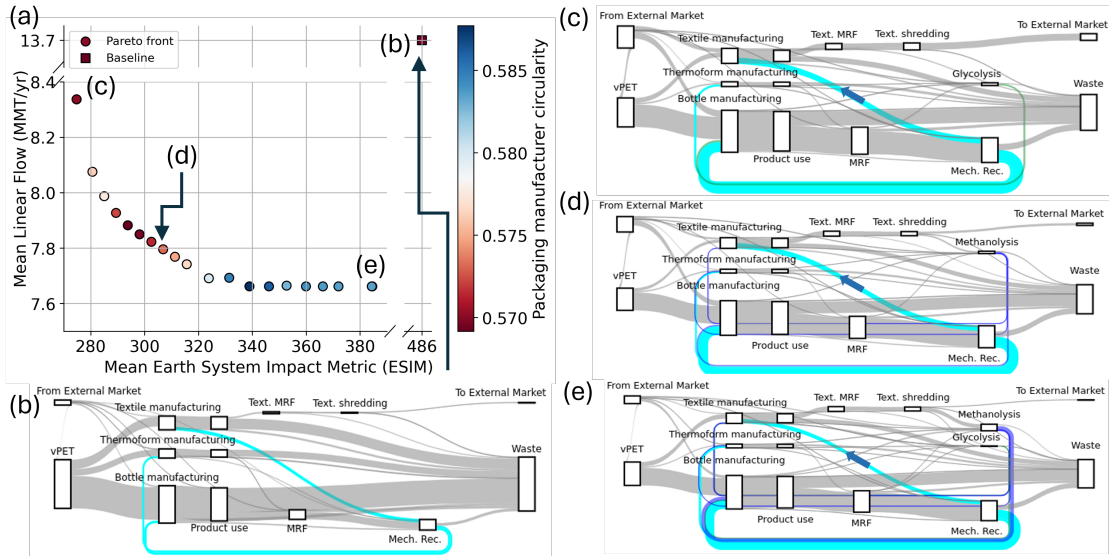


Figure 3: (a) Pareto front showing trade-offs between Mean Linear Flow and Mean ESIM. The Circulytics score of the packaging manufacturer is shown by the color bar but is 0.490 for the baseline, outside the range of the colorbar. Sankey diagrams (b-e) show the relative material flow rates between the different agents for the solutions indicated, with cyan, blue, and green flows denoting recycled material from mechanical recycling, methanolysis, and glycolysis, and all other flows gray. Backward flows are denoted by blue arrows. (b) Baseline linear economy. (c) Minimum Mean ESIM solution. (d) Representative trade-off solution. (e) Minimum Linear Flow solution.

of 10 years. Solution (e) minimizes the Mean Linear Flow by mechanically recycling packaging and “up-cycling” textiles into packaging via methanolysis-based chemical recycling. This is because downcycling does not displace the use of virgin material used for textile production, while methanolysis does. However, methanolysis requires additional processing steps after sorting and shredding, leading to a larger environmental impact. The trade off solutions are similar to (d) combine the pathways in different proportions. However, all trade-off solutions dominate the baseline (b).

As shown by the color bar in **Figure 3a**, although improved network-level circularity generically leads to improved agent-level circularity, the reverse is not always true. The solutions that maximize the packaging and textile manufacturer’s Circulytics scores and the Pareto front of trade-off solutions balancing the objectives are shown in **Figure 4**. The packaging manufacturer’s circularity is maximized by solution (d) when it sources most input material from waste textiles and packaging via methanolysis, but the textile manufacturer produces an excess of textiles, which are disposed of. This is because the resulting post-industrial scrap can be recycled and used by the packaging manufacturer, increasing their circularity level. However, the textile manufacturer’s circularity can be improved significantly at only a small cost to the packaging manufacturer’s circularity by solution (e) if there is less excess production and recycled textile material is diverted from packaging to textiles. Once all of the recycled textile material is used for textile production, the textile manufacturer can improve their circularity even more by diverting recycled packaging material from packaging, but this comes at a larger cost to the packaging manufacturer’s circularity. Finally, the textile manufacturer’s circularity is maximized by solution (f) when no consumer reuse occurs and the packaging manufacturer produces an excess of product that ends up being discarded, since the resulting post-industrial scrap and post-consumer waste can be recycled and used by the textile manufacturer. Similarly to the maximum packaging manufacturer circularity solution, this only improves the textile circularity marginally while significantly reducing the packaging manufacturer’s circularity and NPV. Because of this, although the trade-off solutions are more circular than the baseline, the single-objective manufacturer circularity solutions are less circular, and as shown by the color code, all of the solutions have a larger environmental impact than the baseline.

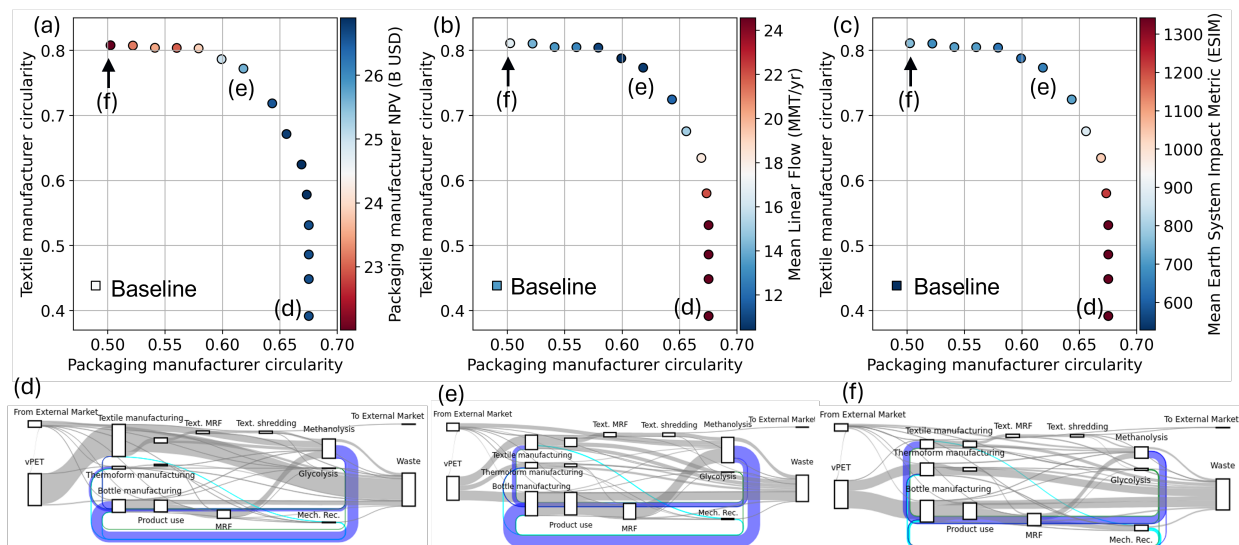


Figure 4: Pareto front showing trade-off solutions that balance the packaging and textile manufacturer's Circulytics scores, which are shown on the x-axis and y-axis. The baseline is indicated by the square. The color bars in (a-c) indicate the NPV of the packaging manufacturer, Mean Linear Flow, and Mean ESIM. Sankey diagrams (d-f) show the optimal packaging manufacturer circularity solution, a representative trade-off solution, and optimal textile manufacturer circularity solution.

Conclusions & Recommendations

In conclusion, we find that for the PET plastic supply chain, improvements in one agent's circularity may come at the expense of other agents' circularity or network-level circularity due to loopholes in circularity assessment frameworks. Furthermore, improved agent- and network-level circularity do not necessarily translate to lower environmental impacts. Therefore, in future work we aim to develop improved agent-level circularity indicators that avoid burden-shifting.

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References

- [1] Ellen MacArthur Foundation, Circulytics- Method Introduction, Indicators, Definitions, Industry Classification, 2022.
- [2] Wang, S., Maravelias, C.T., Optimization methods for plastics management supply chain design. *AIChE Journal*, 70, 8, 2024.
- [3] Chaudhari, U. S., Patil, A., Hossain, T., Watkins, D. W., Hartley, D. S., Reck, B. K., Handler, R. M., Johnson, A. T., Thompson, V. S., Shonnard, D. R., Minimum GHG emissions and energy consumption of U.S. PET and polyolefin packaging supply chains in a circular economy. *RSC Sustain.*, 3, 7, 2025.
- [4] Badejo, O., Hernández, B., Ierapetritou, M. Design of the Transition for Sustainable Plastic Waste Management under Carbon Policies in the United States. *Ind. Eng. Chem. Res.*, 64, 10, 2025.

- [5] Munoz-Briones, P. A., del Carmen Munguía-López, A., Sanchez-Rivera, K., Avraamidou, S., Integrated decision-making approach for the simultaneous design of food packaging and waste management technologies to achieve a Circular Economy. *Computers & Chemical Engineering*, 202, 109269, 2025.
- [6] Ahmed, A., Nair, A., Torres, A. I., Design and optimization of circular economy networks—A case study of PET. *Computers & Chemical Engineering*, 200, 109164, 2025.
- [7] Thakker, V., Bakshi, B. R., Designing Value Chains of Plastic and Paper Carrier Bags for a Sustainable and Circular Economy. *ACS Sustainable Chemistry & Engineering*, 9, 49, 2021.
- [8] Thakker, V., Bakshi, B. R., Toward sustainable circular economies: A computational framework for assessment and design. *J. Clean. Prod.*, 295, 126353, 2021.
- [9] Pert, D., Torres, A. I., A Framework for Dynamic Modeling of Circular Economy Networks: The Polyethylene Terephthalate (PET) Packaging Supply Chain as a Case Study. *Ind. Eng. Chem. Res.*, 64, 22, 2025.
- [10] Rockström, J., Steffen, W. et al, Planetary Boundaries: Exploring the Safe Operating Space for Humanity. *Ecology and Society*, 14, 2, 2009.
- [11] Steffen, W., Richardson, K. et al, Planetary boundaries: Guiding human development on a changing planet. *Science*, 347, 1259855, 2015.
- [12] Ryberg, M. W., Owsianiak, M., Richardson, K., Hauschild, M. Z., Development of a life-cycle impact assessment methodology linked to the Planetary Boundaries framework. *Ecol. Indic.*, 88, 2018.
- [13] Baratsas, S. G., Pistikopoulos, E. N., Avraamidou, S., A quantitative and holistic circular economy assessment framework at the micro level. *Computers & Chemical Engineering*, 160, 107697, 2022.
- [14] World Business Council for Sustainable Development, Circular Transition Indicators (CTI) V4.0: Metrics for Business, <https://coilink.org/20.500.12592/m4z80w>, 2023.
- [15] Ellen MacArthur Foundation, Circularity Indicators: An approach to measuring circularity, <https://www.ellenmacarthurfoundation.org/material-circularity-indicator>, 2019.
- [16] Kondili, E., Pantelides, C. C., Sargent, R. W. H., A general algorithm for short-term scheduling of batch operations—I. MILP formulation. *Computers & Chemical Engineering*, 17, 2, 1993.
- [17] Chaudhari, U. S., Lin, Y., Thompson, V. S., Handler, R. M., Pearce, J. M., Caneba, G., Muhuri, P., Watkins, D., Shonnard, D. R., Systems Analysis Approach to Polyethylene Terephthalate and Olefin Plastics Supply Chains in the Circular Economy: A Review of Data Sets and Models. *ACS Sustain. Chem. Eng.*, 9, 22, 2021.
- [18] Chaudhari, U. S., Watkins, D. W., Handler, R. M., Reck, B. K., Johnson, A. T., Hossain, T., Hartley, D. S., Thompson, V. S., Shonnard, D. R., Environmental and socio-economic Pareto-front trade-off analysis of U.S. PET packaging material in a circular economy. *Sustain. Prod. Consum.*, 60, 2025.
- [19] NAPCOR, 2020 PET Recycling Report, https://napcor.com/wp-content/uploads/2023/12/NAPCOR_2020RateReport_FINAL.pdf, 2021.
- [20] Hernández, B., Vlachos, D. G., Ierapetritou, M. G., Superstructure optimization for management of low-density polyethylene plastic waste. *Green Chem.*, 26, 17, 2024.
- [21] Walzberg, J., Frayret, J. M., Eberle, A. L., Carpenter, A., Heath, G., Agent-based modeling and simulation for the circular economy: Lessons learned and path forward. *J. Ind. Ecol.*, 27, 5, 2023.
- [22] Alumur, S. A., Nickel, S., Saldanha-da-Gama, F., Verter, V., Multi-period reverse logistics network design. *European Journal of Operational Research*, 220, 1, 2012.
- [23] King, S., Weedon, G., Embodiment is ecological: The metabolic lives of whey protein powder. *Body & Society*, 26, 1, 2020.

- [24] Rebitzer, G., Ekvall, T., Frischknecht, R., Hunkeler, D., Norris, G., Rydberg, T., Schmidt, W., Suh, S., Weidema, B. P., Pennington, D. W., Life cycle assessment: Part 1: Framework, goal and scope definition, inventory analysis, and applications. *Environment International*, 30, 5, 2004.
- [25] Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., Weidema, B., The ecoinvent database version 3 (part i): Overview and methodology. *Int J Life Cycle Assess*, 21, 9, 2016.
- [26] Bare, J., Traci 2.0: The tool for the reduction and assessment of chemical and other environmental impacts 2.0. *Clean Technologies and Environmental Policy*, 13, 5, 2011.
- [27] Xue, Y., Bakshi, B. R., Metrics for a nature-positive world: A multiscale approach for absolute environmental sustainability assessment. *Science of The Total Environment*, 846, 157373, 2022.
- [28] Lade, S. J., Steffen, W., De Vries, W., Carpenter, S. R., Donges, J. F., Gerten, D., Hoff, H., Newbold, T., Richardson, K., Rockström, J., Human impacts on planetary boundaries amplified by Earth system interactions. *Nat Sustain*, 3, 2, 2019.
- [29] Lade, S. J., Fetzer, I., Cornell, S. E., Crona, B., A prototype Earth system impact metric that accounts for cross-scale interactions. *Environ. Res. Lett.*, 16, 11, 2021.
- [30] GreenBlue, Chemical Recycling: Making Fiber-to-Fiber Recycling a Reality for Polyester Textiles, <https://greenblueorg.s3.amazonaws.com/smm/wp-content/uploads/2018/05/Chemical-Recycling-Making-Fiber-to-Fiber-Recycling-a-Reality-for-Polyester-Textiles-1.pdf>, 2018.
- [31] Uekert, T., Singh, A., DesVeaux, J. S., Ghosh, T., Bhatt, A., Yadav, G., Afzal, S., Walzberg, J., Knauer, K. M., Nicholson, S. R., Beckham, G. T., Carpenter, A. C., Technical, Economic, and Environmental Comparison of Closed-Loop Recycling Technologies for Common Plastics. *ACS Sustain. Chem. Eng.*, 11, 3, 2023.
- [32] Resource Recycling, Thermoform recycling realities, <https://resource-recycling.com/recycling/2021/07/20/thermoform-recycling-realities/>, 2021.
- [33] U.S. Environmental Protection Agency, Advancing Sustainable Materials Management: 2018 Fact Sheet, <https://www.epa.gov/facts-and-figures-about-materials-waste-and-recycling/advancing-sustainable-materials-management>, 2020.
- [34] Hart, W. E., Watson, J.P., Woodruff, D. L., Pyomo: Modeling and solving mathematical programs in python. *Mathematical Programming Computation*, 3, 3, 2011.
- [35] Bynum, M. L., Hackebeil, G. A., Hart, W. E., Laird, C. D., Nicholson, B. L., Sirola, J. D., Watson, J.P., and Woodruff, D. L., *Pyomo – optimization modeling in python*, Springer, 2021.
- [36] Wächter, A., Biegler, L. T., On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. *Mathematical programming*, 106, 1, 2006.
- [37] Nicholson, B., Sirola, J. D., Watson, J.P., Zavala, V. M., Biegler, L. T., Pyomo.dae: A modeling and automatic discretization framework for optimization with differential and algebraic equations. *Math. Prog. Comp.*, 10, 2, 2018.
- [38] Mavrotas, G., Effective implementation of the ϵ -constraint method in Multi-Objective Mathematical Programming problems. *Applied Mathematics and Computation*, 213, 2, 2009.

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