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Design and Optimization of Circular Economy Networks: A Case Study of Polyethylene Terephthalate (PET)

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ABSTRACT

Circular systems design is an emerging approach for promoting sustainable development. Despite its perceived advantages, the characterization of circular systems remains loosely defined and ambiguous. This work proposes a network optimization framework that evaluates three objective functions related to economic and environmental domains and employs a Pareto analysis to illuminate the trade-offs between objectives. The US polyethylene terephthalate (PET) value chain is selected as a case study and represented via a superstructure containing various recycling pathways. The superstructure optimization problems are modeled as a mixed integer linear program (MILP) and linear programs (LPs), implemented in Pyomo, and solved with CPLEX for a one-year assessment horizon. Solutions to the circular economy models are then compared to the corresponding solutions of linear economy models. Preliminary results show that the optimal circular network is advantageous over the optimal linear network for all objectives subject to the current market supply of raw materials and the total cost of production. However, when considering the present chemical processing infrastructure of the US economy and unrestricted biomass feedstock availability, a linear economy is favorable as an outcome of low operating cost and carbon sequestration.

Keywords: Circular Economy, Supply Chain Optimization, Sustainability, Plastic Recycling

INTRODUCTION

With the growth of modern societies, waste management and finite resource depletion have become problematic. A primary facilitator of this phenomenon is the extensive employment of linear systems where materials are extracted, used, and discarded. Due to heightened concerns regarding finite resource depletion and the environmental effects of mismanaged waste, there is growing interest in adopting circular economies. A circular economy (CE) strives to eliminate waste and pollution, circulate products and materials at their highest level, and regenerate nature [1]. Applications of a CE have been present, to some extent, at the micro-level of some organizations. However, what remains elusive is effective representation at the macro-level and well-defined metrics and methodologies for achieving and quantifying circularity.

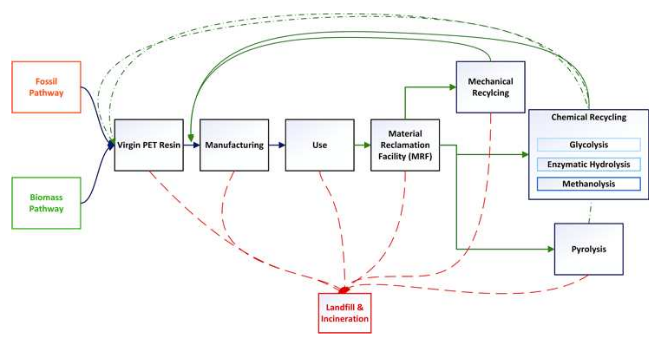


Figure 1. High-level superstructure representation.

Each year, plastics constitute roughly 400 million tonnes of generated waste, of which approximately 80% enters landfills or is emitted into the environment [2]. Of all produced plastics, polyethylene terephthalate (PET) is one of the most widely consumed, with applications of PET ranging from consumer packaging to films and textiles (polyester). In the US, historical demands for polyester and bottle-grade PET comprise over 85% of all PET products [3]. However, recycling rates for bottles and general textiles are approximately 30% and 15%, respectively [4,5]. For these reasons, we consider the PET economy as an application case study for assessment.

A holistic representation of the PET value chain (product life cycle) and potential circular processing pathways is depicted in Figure 1. The analysis is posed as a superstructure optimization problem. The superstructure includes fossil and biomass feedstocks for PET precursors, production routes from these precursors to virgin PET (vPET), manufacturing and use phases for PET-based products, and end-of-life (EoL) processing technologies. EoL processes include traditional and novel processing of the following grouping: landfilling, incineration, mechanical recycling (MR), chemical recycling (CR), and thermochemical recycling.

The application of various recycling processes allows for material retention within the value chain. However, it remains unclear how favorable these processes are over a dominantly linear PET economy. To enhance this understanding, we formulate a mixed integer linear programming problem (MILP) where we assess an economic, environmental, and material utilization objective. The optimization problems are solved to determine the optimal selection of processing technologies and material flows that satisfy demand and are then compared to the optimal solutions of a linear economy reference model. The linear reference model is obtained by imposing flow restriction constraints, which void recycle flows. A Pareto analysis is then performed using the epsilon-constrained method defined in [6] to identify the trade-offs between the objectives.

METHODS

Modeling Framework

For modeling purposes, a State Task Network (STN) formulation where processes (tasks) consume and produce materials (states) is followed. Two types of nodes are defined, one constituting key chemical components and the other technologies that convert components. Technology nodes (j) accept flows from component nodes, performing composition transformations and acting as the influx to other component nodes. Component nodes (i) combine fluxes from different technology nodes and are also connected to the external market, allowing purchases and sales of material. The characterization of the nodes is depicted in Figure 2. A technology matrix (A) is defined to contain process conversion information representing transformations across technology nodes. The technology matrix is informed by industrial data and process simulations from the literature.

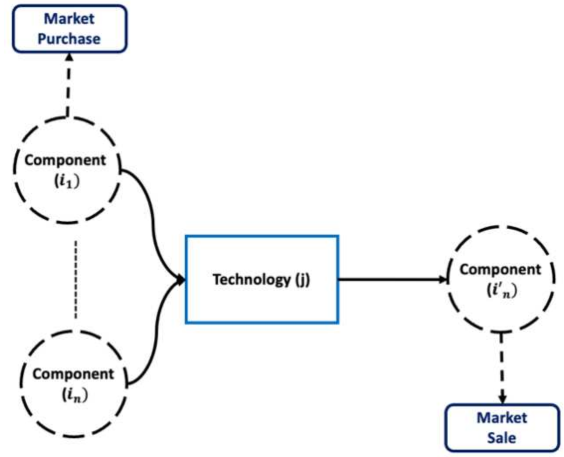


Figure 2. Network node characterization.

The generalized model equations for the given framework are defined by equations (1-7). Eqs. (1) and (2) define the generation and consumption of component i in technology j. Where γ_{ij}, a conversion factor, is positive for generative transformations and negative for consumption. Parameter γ_{ij} constitutes the members of matrix (A) and is defined by industrial data aggregated by Franklin Associates [7], the US EIA [8], the US EPA [9], and Aspen simulations documented in the literature [10-17]. Variable l_j represents the total flow through a technology node. Sets J^G and J^C designate producing and consuming technology nodes, respectively.

$$g_{ij} = \gamma_{ij} l_j \qquad \forall i \in I, \forall j \in J^G \qquad (1)$$

$$c_{ij} = -\gamma_{ij} l_j \qquad \forall i \in I, \forall j \in J^C \qquad (2)$$

$$\sum_{j \in J} \gamma_{ij} l_j + p_i = s_i \qquad \forall i \in I \qquad (3)$$

Eq. (3) represents the general material balance for all components in the set I, stating that the purchase plus the total generation and consumption of i across the set of technologies (J) is equal to the market sales or excess of i. Furthermore, component purchases (p_i) are bounded by an upper limit (p_i^L), which in this analysis is the five-year historical average supply for all raw materials. Eq. (5) states that the demand for end products must be satisfied for all I belonging to a subset I^D. Table 1 represents the annual rate of PET consumption (megaton) in the US in 2018 [3,18].

$$p_i \le p_i^L \qquad \forall i \in I \qquad (4)$$

$$\sum_{j \in J^G} g_{ij} \ge \mathrm{d_i} \qquad \forall i \in I^D \qquad (5)$$

$$g_{ij'} \le \eta_i \sum_{j \in J^G} g_{ij} \qquad \forall i \in I^G \qquad (6)$$

$$c_{ij'} \le \eta_i \sum_{j \in J^C} c_{ij} \qquad \forall i \in I^C \qquad (7)$$

Lastly, Eqs. (6-7) generalizes the process constraints imposed on network flows to satisfy select technical requirements. These equations state that the production or consumption of component i by j is limited by the net generation or consumption of i multiplied by a scalar η_i. The parameter η_i represents flow ratios and corresponds to current process capabilities detailed in the literature. I^G and I^C, are subsets of I. And j' is a referenced technology node corresponding to η_i. For example, one such constraint is the allowable composition of mixed virgin PET resin and recycled PET (rPET) resin produced by mechanical recycling that satisfies intrinsic viscosity requirements for processing into new bottles. Here, η_i is 0.35 [19] and j' is the mechanical recycling of post-use bottles. Additional technical constraints include an upper bound on the fraction of end-of-life textiles (EoL) to be downcycled to satisfy a portion of demand. Secondly, there is an upper bound on the amount of non-bottle/non-polyester EoL materials that can be recycled, which discounts products that generally cannot be recycled, such as food containers.

Table 1: Case study demand specification.

Product Type	Demand (Mt/year)
Bottles	2.84
Polyester	7.84
Films/sheets/others	1.17

Design Objectives

Three design objectives are assessed to explore economic and environmental domains. These include total annualized cost of production, process greenhouse gas emissions (GHGs), total virgin raw material utilization.

Total Annualized Cost

$$TAC = \sum_{j\in J^E}(opex_j l_j + ACCR\sum_{t\in T} capex_{jt}) \qquad (8)$$

The economic dimension is evaluated with Eq. (8) which states that the total annualized cost of production is equal to the sum of operational costs and annualized capital expenses (ACC) for the technologies. Operating cost ($opex_j$) equals the sum of feed, utility, and labor minus the sale of by-products for each j. We assume a ten-year amortization period and an interest rate of 15%, which correlates to an annual capital charge ratio (ACCR) of 0.199 [20]. Investment costs ($capex_{jt}$) are indexed by plant (t) belonging to the set of plants (T). Set J^E is a subset of economically evaluated technologies.

$$\frac{capex_j^{ref}}{\left(capacity_j^{ref}\right)^{0.6}}\left[a^{0.6} + \frac{b^{0.6}-a^{0.6}}{b-a}\left(capacity_{jt} - az_{jt}\right)\right] \qquad (9)$$

$$capacity_{jt} \le Mz_{jt} \qquad \forall j \in J, \forall t \in T \qquad (10)$$

$$l_j \le \sum_{t\in T} capacity_{jt} \qquad \forall j \in J \qquad (11)$$

To account for economies of scale, the six-tenths rule is applied to estimate $capex_{jt}$. This rule leads to a non-linear non-convex equality. Thus, a secant linearization [21] as presented in Eq. (9) is applied, where a and b are lower and upper bounds of the approximating function. $capex_j^{ref}$ and $capacity_j^{ref}$ are reference parameters taken from the literature. And the capacity of plant t for process j is represented by $capacity_{jt}$. Furthermore, the binary variable z_{jt} indicates whether a plant t is selected for the process j. Eq. (10) ensures that capacity is zero if plant t of process j is not selected, with M equal to the maximum plant capacity. Lastly, Eq. (11) bounds net flow through j by the total capacity of j.

GHG Emissions

$$GHG = \sum_{j\in J^E}\phi_j g_{ij} \qquad \forall i \in I^R \qquad (12)$$

The environmental objective presented by Eq. (12) represents raw material extraction, processing, and manufacturing emissions. It states that the net greenhouse gas (GHG) emissions are equal to the total generation of components i in the set of reference products I^R multiplied by the emission factor ϕ_j which measures carbon equivalents (CO_2e). Set I^R is defined such that emission parameters are normalized per reference product belonging to each evaluated technology node. The considered GHGs are carbon dioxide, methane, and nitrous oxide. Parameter ϕ_j is determined with process data available in the literature.

Virgin Raw Material Utilization

$$VF = \sum_{i\in I^F} p_i \qquad (13)$$

The final design goal considers raw material use and measures network material efficiency. This objective serves as a proxy for quantifying circularity. The objective function is defined by Eq. (13) and represents the sum of market purchases of virgin feedstock, where I^F describes feedstock components.

Optimization Problem

The analysis involves solving the optimization problem defined in Eq. (14). Here, Z represents each objective function, where Eq. (14) is a MILP for the annualized cost objective but an LP for both environmental and material use objectives as Eq. (9-11) pertain only to the economic problem.

$$\begin{aligned} &\min Z \\ &s.t. Eq.(1-7), Eq(9-11) \qquad (14) \\ &l_j, s_i, p_i, capex_{jt}, capacity_{jt} \ge 0, z_{jt} \in \{0,1\} \end{aligned}$$

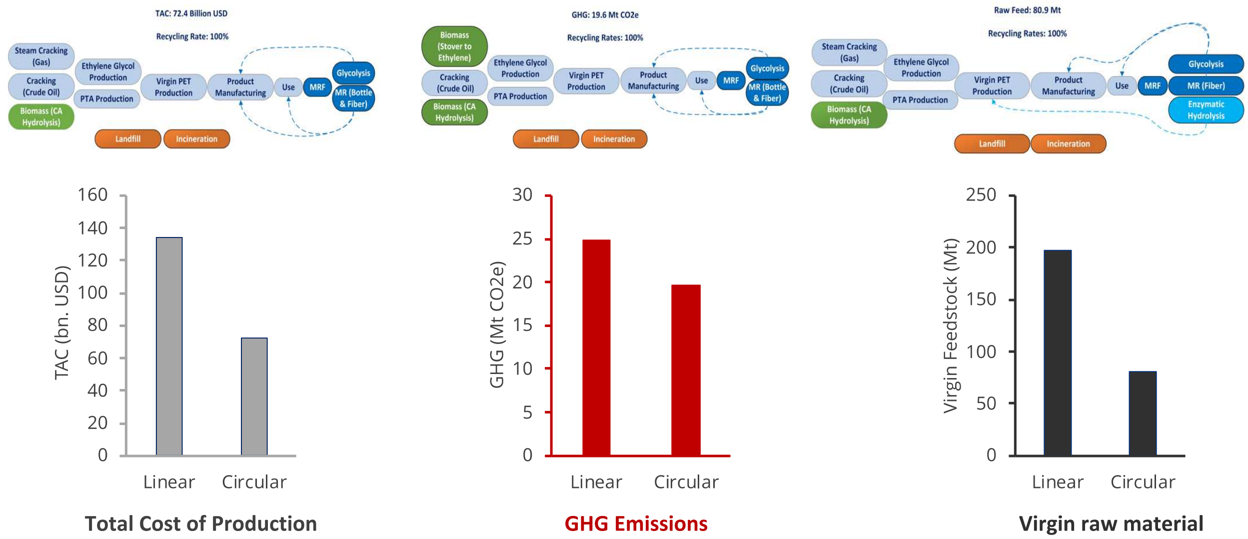


Figure 3. Comparison of single objective solutions of linear reference model and design model with the resultant dominant network configurations. MR represent mechanical recycling of bottles and downcycling of polyester.

RESULTS

Single-Objective Solutions

The optimization problem is solved using CPLEX version 22.1.1 and Pyomo, a Python optimization modeling language [22]. The results and comparisons for the single objective problems are presented in Figure 3. Considering the economic objective, the optimal network configuration of the design model is circular, employing both mechanical recycling and glycolysis. Final products from recycling include rPET that is sent directly to the manufacturing stage to create final PET end products. Comparing this optimal network to the solution of the corresponding linear reference model shows that a circular network offers a 46% cost reduction over the linear counterpart.

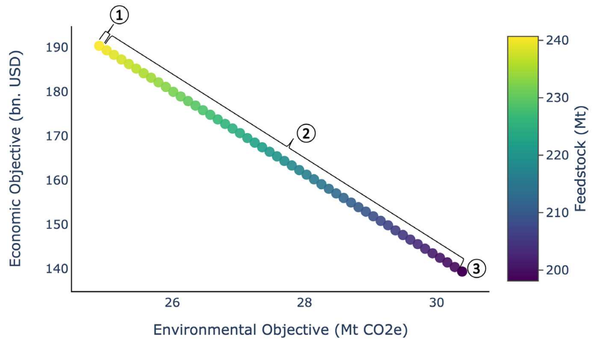
Likewise, for the GHG emission objective, the solution of the design model leads to a circular network achieved with mechanical recycling and glycolysis. However, contrary to the network configuration of the economic objective, more biomass feedstock is used over fossil feedstock. Additionally, comparing the solution of the GHG objective to the corresponding linear reference gives a 21% reduction in supply chain process emissions. This reduction is lower relative to that achieved by the economic objective.

Lastly, the solution of the circular design model for the virgin raw material objective is a circular network with a 59% reduction in raw material consumption. However, compared to the previous design solutions, this network consists of a much higher application of chemical recycling via glycolysis and enzymatic hydrolysis and the rest of the downcycling of polyester. In addition to rPET production, monomers are produced and sent upstream for polymerization into PET.

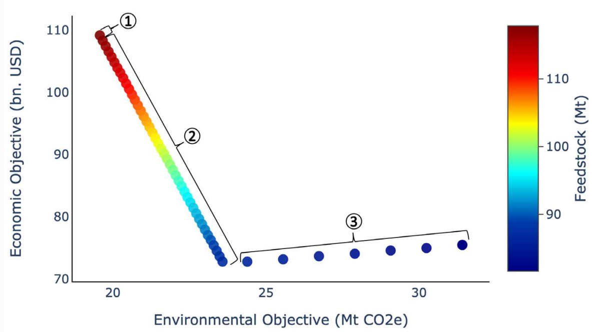
In addition to the base cases, additional considerations are evaluated for the economic and environmental objectives. The first assigns zero Capex to developed US processes to account for existing infrastructure. The resultant networks for both linear and circular models converge to an equivalent linear network. The selected network utilizes a purely fossil-based pathway employing steam cracking of natural gas and cracking of crude oil. The second consideration is unrestricted access to all feedstock, where unlimited is defined by altering market bounds to allow one gigatonne for all feed components. Like the first consideration, solving the reference and circular model leads to an equivalent linear network. However, contrary to the previous network, the obtained network follows a purely biomass-based pathway via biomass-to-ethylene conversion and acid hydrolysis of biomass to produce paraxylene.

Pareto Assessment

The Pareto fronts for the design and linear models are shown in Figure 4. The linear model exhibits a linear trade-off between all objectives, where reducing emissions leads to higher-cost networks that consume more virgin feedstock. This trend occurs as increasing biomass feed consumption leads to reduced emissions. Yet, because process conversions of biomass processes are relatively low compared to fossil processes, higher raw material input is required to satisfy demand. These observations are further validated via the change in configuration of the selected optimal networks numbered in Figure 4.



(a) Linear reference network



(b) Circular network

Figure 4. Pareto front with network distinctions for linear model (a) and circular model (b).

In Figure 4(a), network one corresponds to the solution of the GHG emission objective presented in Figure 3 without selections for recycling. Likewise, network three is consistent with the cost objective network in Figure 3, without recycling. Network two corresponds to an intermediary of network one with steam cracking of natural gas without recycling, supporting the observable transition from biomass pathways to better conversion fossil pathways.

For the circular model, the Pareto front is piecewise linear. As shown in Figure 4(a), the leftmost trend line abides by the reasoning discussed for the linear model. However, after some threshold, attaining increased material circularity (lesser virgin feedstock consumption) leads to more emissions and higher annualized costs. The rationale for this behavior is that further reductions in material consumption demand a reasonably material-efficient network. Such a network is achievable by selecting more chemical recycling processes, contributing to increased capital investment and GHG emissions. Like the linear model, these trends are supported by the network configurations spanning the Pareto front. Looking at Figure 4(b), network three corresponds to the solution of the virgin raw material objective presented in Figure 3, plus the mechanical recycling of bottles. Network one corresponds to the GHG emission objective in Figure 3. And network two, an intermediary of network one with steam cracking of natural gas.

CONCLUSIONS

This work formulates a superstructure optimization problem for the US polyethylene terephthalate value chain to determine an optimal network selection consisting of processing technologies and material flow pathways satisfying each design goal for a one-year assessment period. The three assessed design goals are total annualized cost, GHG process emissions, and virgin feedstock consumption, which served as a proxy for measuring material circularity. Finally, a multi-objective Pareto assessment was performed to illuminate existing trade-offs between competing objectives for the linear and circular design models.

The results of the single-objective analysis indicate that circular PET supply chains offer lower GHG process emissions, water consumption, and virgin feedstock usage. Additionally, under current market conditions, a circular PET network is a better investment than a linear network when constructed from a zero-infrastructure ground state. Next, the results of the Pareto assessment portray a linear trade-off between objectives for the linear model, with a correlation between total annualized cost and virgin feedstock consumption, which vary inversely with GHG process emissions. The same observation is initially present for the circular model. However, attaining better material circulation increases the carbon intensity and cost for the selected networks, chiefly due to the additional processing technologies required to realize greater network efficiency.

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