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1 **Environmental and Socio-economic Pareto-front Trade-off Analysis of U.S. PET Packaging**
2 **Material in a Circular Economy**

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5
6 **Abstract**

7 Various recycling technologies are emerging to implement circular economy in plastics supply
8 chain systems. However, the environmental and socio-economic trade-offs of plastics in circular
9 economy are not well understood at a systems level. Particularly, quantifying these trade-offs as a
10 function of end-of-life (EOL) management decisions, including transition of recycling
11 technologies, systems level metrics such as circularity, recycled content, and the need for fossil-
12 derived plastics are not well understood. The present study addressed these research gaps by
13 applying a systems analysis modeling approach that utilizes material flow analysis, life cycle
14 assessment, socio-economic data, and system optimization techniques for polyethylene
15 terephthalate (PET) packaging supply chains in the United States. Pareto-front trade-offs between
16 conflicting environmental and socio-economic impacts as well as those between socio-economic
17 impacts and circularity were explored using the epsilon constraint method. The Pareto-front trade-
18 off analysis revealed the transition of EOL management strategies for PET packaging systems,
19 including changes in selection of recycling technologies, to aid decision making process by
20 quantifying studied system metrics. Transitioning from environmentally optimal to socio-
21 economically optimal systems led to increased employment (by 17%), wages (by 26%), and
22 revenues (by 6%) but also led to increased global warming potential (GWP; by 65%), energy
23 consumption (by 59%), and reliance on fossil PET in the system (by 78%). Finally, the results
24 show that there is not a unique set of recycling technologies to achieve a sustainable circular
25 economy of PET packaging system, instead it depends on the decision maker's objectives and
26 targeted metrics of the system.

27

1 **Keywords:** Sustainability, Circular Economy, Optimization, Trade-offs, Waste plastics, Socio-
 2 economics

3 **Nomenclature**

Abbreviation	Description
ABM	Agent based modeling
BFA	Brute force algorithm
BHET	Bis-2-hydroxyethyl terephthalate
CED	Cumulative energy demand
CFR	Collection for recycling
CO ₂ -eq	Carbon dioxide equivalent
DMT	Dimethyl terephthalate
EOL	End-of-life
EPA	Environmental protection agency
GFRP	Glass reinforced plastic
GHG	Greenhouse gases
GWP	Global warming potential
IPCC	Intergovernmental panel on climate change
ISBM	Injection stretch blow molding
LCA	Life cycle assessment
LCIA	Life cycle impact assessment
LP	Linear programming
MCDA	Multicriteria decision analysis
MFA	Material flow analysis
MILP	Mixed integer linear programming
MIO	Mixed input output
MJ	Mega joules
MMT	Million metric tons
MRF	Material recovery facility
MT	Metric tons
NAICS	North American industry classification system
NLP	Nonlinear programming
PCI	Plastics circularity index
PE	Polyethylene
PET	Polyethylene terephthalate
PJ	Peta joules
PP	Polypropylene
RHS	Right hand side
SBDP	Solvent-based dissolution precipitation
TPA	Terephthalic acid
UGFRP	Upcycling to glass fiber reinforced plastic
UNEA	United Nations environment assembly
U.S.	United States
USD	United States Dollar
V-PET	Virgin polyethylene terephthalate
WtE	Waste-to-energy
WTP	Willingness-to-pay

4

Symbol	Description	Unit
Virgin PET Resin Production		
Parameters		
E_0	CED LCIA factor for virgin PET production	MJ/kg
ε_0	GWP LCIA factor for virgin PET production	MT CO ₂ -eq/MT
P_0	Employment factor for virgin PET production	Employee/MT
R_0	Revenue factor for virgin PET production	Revenue/MT
S_0	Wage factor for virgin PET production	Wage/MT
Variable		
X_0	Amount of virgin PET resin	MT
ISBM		
Parameters		
E_1	CED LCIA factor for ISBM	MJ/kg
ε_1	GWP LCIA factor for ISBM	MT CO ₂ -eq/MT
P_1	Employment factor for ISBM	Employee/MT
R_1	Revenue factor for ISBM	Revenue/MT
S_1	Wage factor for ISBM	Wage/MT
w_1	Yield loss factor for ISBM	%
Variables		
X_1	Input material flow to ISBM	MT
X_3	Output material flow from ISBM after accounting for yield loss	MT
Film/Sheet/Others extrusion		
Parameters		
E_2	CED LCIA factor for film/sheet/others extrusion	MJ/kg
ε_2	GWP LCIA factor for film/sheet/others extrusion	MT CO ₂ -eq/MT
P_2	Employment factor for film/sheet/others extrusion	Employee/MT
R_2	Revenue factor for film/sheet/others extrusion	Revenue/MT
S_2	Wage factor for film/sheet/others extrusion	Wage/MT
w_2	Yield loss factor for film/sheet/others extrusion	%
Variables		
X_2	Input material flow to film/sheet/others extrusion process	MT
X_4	Output material flow from film/sheet/others extrusion process after accounting for yield loss	MT
Landfill		
Parameters		
E_3	CED LCIA factor for landfilling	MJ/kg
ε_3	GWP LCIA factor for landfilling	MT CO ₂ -eq/MT
P_3	Employment factor for landfilling	Employee/MT
R_3	Revenue factor for landfilling	Revenue/MT
S_3	Wage factor for landfilling	Wage/MT
Variable		
X_5	Input material flow to landfill	MT
Incineration with energy recovery / WtE		
Parameters		

E_4	CED LCIA factor for WtE	MJ/kg
ε_4	GWP LCIA factor for WtE	MT CO ₂ -eq/MT
P_4	Employment factor for WtE	Employee/MT
R_4	Revenue factor for WtE	Revenue/MT
S_4	Wage factor for WtE	Wage/MT
Variable		
X_6	Input material flow to WtE	MT
MRF		
Parameters		
E_5	CED LCIA factor for MRF	MJ/kg
ε_5	GWP LCIA factor for MRF	MT CO ₂ -eq/MT
P_5	Employment factor for MRF	Employee/MT
R_5	Revenue factor for MRF	Revenue/MT
S_5	Wage factor for MRF	Wage/MT
w_3	Yield loss factor for MRF	%
Variables		
X_7	Input material flow to MRF	MT
X_8 to X_{12}	Output material flow from MRF after accounting for yield loss to various recycling technologies	MT
Mechanical Recycling		
Parameters		
E_6	CED LCIA factor for mechanical recycling	MJ/kg
ε_6	GWP LCIA factor for mechanical recycling	MT CO ₂ -eq/MT
P_6	Employment factor for mechanical recycling	Employee/MT
R_6	Revenue factor for mechanical recycling	Revenue/MT
S_6	Wage factor for mechanical recycling	Wage/MT
w_4	Yield loss factor for mechanical recycling	%
Variables		
X_8	Input material flow to mechanical recycling	MT
X_{13}	Output material flow from mechanical recycling after accounting for yield loss	MT
Dissolution		
Parameters		
E_7	CED LCIA factor for dissolution	MJ/kg
ε_7	GWP LCIA factor for dissolution	MT CO ₂ -eq/MT
P_7	Employment factor for dissolution	Employee/MT
R_7	Revenue factor for dissolution	Revenue/MT
S_7	Wage factor for dissolution	Wage/MT
w_5	Yield loss factor for dissolution	%
Variables		
X_9	Input material flow to dissolution	MT
X_{14}	Output material flow from dissolution after accounting for yield loss	MT
Glycolysis		
Parameters		
E_8	CED LCIA factor for glycolysis	MJ/kg
ε_8	GWP LCIA factor for glycolysis	MT CO ₂ -eq/MT

P_8	Employment factor for glycolysis	Employee/MT
R_8	Revenue factor for glycolysis	Revenue/MT
S_8	Wage factor for glycolysis	Wage/MT
w_6	Yield loss factor for glycolysis	%
Variables		
X_{10}	Input material flow to glycolysis	MT
X_{15}	Output material flow from glycolysis after accounting for yield loss	MT
Methanolysis		
Parameters		
E_9	CED LCIA factor for methanolysis	MJ/kg
ε_9	GWP LCIA factor for methanolysis	MT CO ₂ -eq/MT
P_9	Employment factor for methanolysis	Employee/MT
R_9	Revenue factor for methanolysis	Revenue/MT
S_9	Wage factor for methanolysis	Wage/MT
w_7	Yield loss factor for methanolysis	%
Variables		
X_{11}	Input material flow to methanolysis	MT
X_{16}	Output material flow from methanolysis after accounting for yield loss	MT
Enzymatic hydrolysis		
Parameters		
E_{10}	CED LCIA factor for enzymatic hydrolysis	MJ/kg
ε_{10}	GWP LCIA factor for enzymatic hydrolysis	MT CO ₂ -eq/MT
P_{10}	Employment factor for enzymatic hydrolysis	Employee/MT
R_{10}	Revenue factor for enzymatic hydrolysis	Revenue/MT
S_{10}	Wage factor for enzymatic hydrolysis	Wage/MT
w_8	Yield loss factor for enzymatic hydrolysis	%
Variables		
X_{12}	Input material flow to enzymatic hydrolysis	MT
X_{17}	Output material flow from enzymatic hydrolysis after accounting for yield loss	MT

1

2 **1. Introduction**

3 The global plastics waste supply chain is 90% linear and only 10% circular (Nordic Council of
4 Ministers; Systemiq 2023). The linear economy (“take-make-use-dispose”) model for plastics
5 represents inefficient use of limited fossil resources resulting from high disposal rates of valuable
6 plastic materials, which further leads to plastic pollution (Bucknall 2020). The costs of damage
7 due to global plastic pollution can range from 13.7 to 282 trillion United States Dollar (USD) if
8 no actions are taken to address the plastics waste problem (Cordier, Uehara et al. 2024). Increased
9 plastic pollution leads to enhanced climate change effects (Wei, Yang and Hedenqvist 2024) and
10 causes environmental, social, and economic damage to nearly all ecosystems (Villarrubia-Gómez,
11 Almroth et al. 2024). Shifting away from the linear economy to a circular economy of plastics is
12 essential to mitigate climate change effects as well as to meet other sustainable development goals
13 (de Sousa 2021).

1 Transition from linear-to-circular economy of plastics could represent a vital environmental,
2 societal, and economic opportunity through efficient management of our valuable resources
3 (Walzberg, Lonca et al. 2021). The goal of such a transition is to minimize our reliance on fossil
4 resources, reduce climate change impacts, generate societal benefits (e.g. employment), and enable
5 economic prosperity, all through synergistic and cooperative partnerships (Ellen MacArthur
6 Foundation 2021). However, linear-to-circular transition requires rethinking of supply chain
7 processes due to changes in material flows (Ellen MacArthur Foundation 2023), often leading to
8 conflicts in achieving these goals (Ahmed, Al-Mohannadi and Linke 2021). Hence, for decision
9 makers to understand these conflicts, a holistic sustainability assessment of plastics material flows
10 is needed to explore the relevant trade-offs of sustainability impacts and their inter-relationships
11 with material flows in a circular economy.

12 Recycling of plastics is one of the important circular economy strategies to save our limited natural
13 fossil resources (Hellweg, Benetto et al. 2023). Between 2018 to 2023, global investments of about
14 USD 190 billion have been made towards increasing circularity in plastics supply chains, and about
15 82% of this total were in the recovery and recycling supply chain processes (The Circulate
16 Initiative 2024). Deployment of various recycling technologies producing high-quality recycled
17 plastic resins has been recognized as an important solution to promote a circular economy in
18 plastics supply chains (Arcà, Reike and Bening 2024, Liu, Barlaz and Johnson 2024).

19 Globally, and in the United States (U.S.), mechanical recycling technology remains the dominant
20 recycling technology for plastics, particularly for polyethylene terephthalate (PET), polyethylene
21 (PE), and polypropylene (PP) plastics. The U.S. represented at least 14% (6.6 million metric tons
22 (MMT)) and 11% (270) of the total global mechanical recycling capacity (48 MMT) and number
23 of recycling plants (2,500), respectively, in 2021 (Friedman 2022). The majority of this total
24 mechanical recycling capacity was equally contributed by PET and PE plastics (Resource
25 Recycling 2022). However, mechanical recycling technology is unable to create virgin-like high
26 quality plastic resins due to degradation of inherent material properties at each recycling loop that
27 affects the strength and appearance of the recycled products (Klotz, Haupt and Hellweg 2022,
28 Bezeraj, Debrje et al. 2025). Due to the lack of supply of high-quality recycled plastics, major
29 consumer goods companies are struggling to achieve their recycled content targets for plastics
30 (World Wildlife Fund (WWF) 2023). Depending on the country and company, the recycled content
31 ranged up to 21% (Brown and Börkey 2024) with an average plastic recycled content of 10-12%
32 (World Wildlife Fund (WWF) 2023).

33 Complementary to mechanical recycling technology, emerging advanced/chemical recycling
34 technologies offer a potential solution to incorporate closed-loop circular economy in plastics
35 supply chains by creating virgin-like high quality plastic resins (America's Plastic Makers® 2022,
36 Kubiczek, Derej et al. 2023). As of 2021 in the U.S., about 45 advanced/chemical recycling plants
37 have been announced with combined planned annual capacities of up to 5 MMT by 2025
38 (Friedman 2022). As these technologies are still in the developing phase, there is a lack of
39 understanding of system-wide sustainability impacts and trade-offs of implementing a closed-loop
40 circular economy in plastics supply chains via emerging advanced/chemical recycling
41 technologies (García-Gutiérrez, Amadei et al. 2025).

1 Our previously developed systems analysis framework enables system-wide assessment of
2 sustainability impacts and trade-offs of alternative/emerging manufacturing technologies
3 compared with traditional business-as-usual technologies relying on fossil resources (Shonnard,
4 Tipaldo et al. 2019, Chaudhari, Lin et al. 2021). The present study utilizes material flow analysis
5 (MFA), life cycle assessment (LCA), socio-economic assessment, and linear programming
6 optimization tools to evaluate the sustainability impacts, trade-offs, and system-level metrics of
7 closed-loop recycling of PET packaging material in the U.S. PET is a suitable plastic for this
8 analysis because it is one of the highest production volume plastic materials in the U.S. and in the
9 world (Nicholson, Rorrer et al. 2021).

10 The U.S. PET material supply chain is unique in terms of its applications, compared to global
11 applications of PET resin (Duan, Wang et al. 2024). Over 85% of the U.S. PET resin is used for
12 packaging applications (e.g. bottles, films, thermoforms) with the remaining 15% used for
13 fiber/textile applications (Nicholson, Rorrer et al. 2021, Chaudhari, Johnson et al. 2022),
14 highlighting the importance of U.S. PET packaging supply chain. On the other hand, over 60% of
15 the global PET material is used for fiber applications (Rorrer, Nicholson et al. 2019). In the U.S.,
16 PET accounts for about 10% of total plastics production (Di, Reck et al. 2021). Due to a short in-
17 use average lifetime (< 1 year) of packaging materials, PET packaging waste alone accounts for
18 about 11% of the total U.S. plastic waste and 27% of the total U.S. plastic containers and packaging
19 waste (U.S. EPA 2020). Moreover, PET packaging waste accounts for about 73% of the total PET
20 material waste generated in the U.S. (U.S. EPA 2020). The systems analysis framework used in
21 our study is limited only to packaging applications of PET material considering sufficient
22 availability of the information and required data to develop the system model.

23 **2. Literature Review**

24 The resolution (5/14) adopted by the United Nations Environment Assembly (UNEA) calls for a
25 holistic approach and highlights the need for conducting environmental and socio-economic
26 assessments related to plastics supply chains (United Nations Environment Programme 2022).
27 Prior literature on circular plastic waste management systems has mainly focused on
28 environmental and economic dimensions of sustainability (De Oliveira, Dantas and Soares 2021,
29 Sandoval-Reyes, He et al. 2024) and lacks socio-economic performance and trade-off evaluation
30 (Haupt and Hellweg 2019, Vanhuyse, Fejzić et al. 2021). Table 1 shows a simplified summary of
31 the identified literature review, mainly related to sustainability assessment of PET packaging
32 material. Detailed review of the identified literature is provided in Section S1 of the Supplementary
33 Information (SI) document.

34

Table 1. Summary of literature review assessing the sustainability of PET plastics in a circular economy

Ref.	Geographical scope	Systems analysis and modeling approach	Environmental impacts	Economic impacts	Socio-economic impacts	Trade-off analysis	Recycling technologies	Blend limit constraint
(Ghosh, Avery et al. 2023)	U.S.	System dynamics, MFA	✓	✓	✗	✗	MR, GL, PY	✗
(Ghosh, Uekert et al. 2023)	U.S.	MFA, ABM, MCDA, BFA	✓	✓	✗	✓	MR, GL, PY, UGFRP	✓
(Pert and Torres 2025)	U.S.	System dynamics	✓	✗	✗	✗	MR	✓
(Ahmed, Nair and Torres 2025)	U.S.	MILP, MFA	✓	✓	✗	✓	MR, GL, EH, MeT, AH, PY	✓
(Gracida-Alvarez, Xu et al. 2023)	U.S.	Scenario analysis	✓	✗	✗	✗	MR, MeT, EH	✗
(Komly, Azzaro-Pantel et al. 2012)	France	NLP	✓	✗	✗	✓	MR, GL	✓
(Andreasi Bassi, Tonini et al. 2021)	Europe	Scenario analysis, MFA	✓	✗	✓	✗	MR	✗
(Cimpan, Bjelle et al. 2023)	Europe	MIO, MFA	✓	✗	✓	✗	MR	✗
(Chin, Lee and Woon 2023)	Malaysia	MILP	✓	✓	✓	✓	MR	✗
(Kuroda, Amasawa et al. 2023)	Japan	LP	✓	✗	✗	✗	MR, PY, GA	✓
(Chaudhari, Lin et al. 2021)	U.S.	MFA, LP	✓	✗	✗	✗	MR, SBDP	✓
(Chaudhari, Patil et al. 2025)	U.S.	MILP, MFA (<i>Geospatial</i>)	✓	✗	✗	✗	MR, SBDP, GL, MeT, EH, PY	✓
(Chaudhari, Watkins et al. 2025)	U.S.	LP	✓	✗	✓	✗	MR, SBDP, GL, MeT, EH	✓
Present study/work	U.S.	LP	✓	✗	✓	✓	MR, SBDP, GL, MeT, EH	✓

1 Notes: MFA: Material flow analysis; ABM: Agent based modeling; MCDA: Multi-criteria decision analysis; BFA: Brute force
2 algorithm; MILP: Mixed integer linear programming; NLP: Non-linear programming; MIO: Mixed input output model; LP: Linear
3 programming; MR: Mechanical recycling; GL: Glycolysis; PY: Pyrolysis; UGFRP: Upcycling to glass fiber reinforced plastic; EH:
4 Enzymatic hydrolysis; MeT: Methanolysis; AH: Alkaline hydrolysis; GA: Gasification; SBDP: Solvent-based dissolution precipitation.

5

6

1 Despite the advances in the field of sustainability assessment of circular plastics supply chains,
2 previously developed system models lack a holistic approach of closed-loop PET packaging
3 material flows in the U.S. with a “cradle-to-cradle” system boundary. For example, prior studies
4 do not specifically include production of virgin resins, semi-manufacturing processes (e.g. blow
5 molding, extrusion etc.), and transportation related steps. Also, there is a need to optimize the
6 system based on socio-economic indicators to determine socio-economic implications of U.S. PET
7 packaging in circular economy. Even though a few studies have conducted Pareto-front trade-off
8 analysis, they lacked socio-economic aspects as well as rigorous Pareto-front analysis to
9 understand the transitions of end-of-life (EOL) management decisions as a function of system
10 metrics and material flows in a circular economy. This hinders the ability of a decision maker to
11 comprehensively understand the material flows and quantify potential trade-offs among
12 sustainability indicators as well as identify alternative circular system designs for plastics.

13 Based on the above-mentioned research gaps and limitations, our previously developed “cradle-
14 to-cradle” PET packaging system model includes major upstream processes such as production of
15 virgin resins and semi-manufacturing processes as well as downstream processes such as
16 conventional EOL disposal processes (e.g. landfill, incineration with energy recovery), existing
17 mechanical recycling technology, and four emerging recycling technologies for PET (Chaudhari,
18 Watkins et al. 2025). In simple words, (Chaudhari, Watkins et al. 2025) developed a system model
19 that determined the optimal EOL management for waste PET packaging waste material with
20 minimum environmental impacts and maximum socio-economic benefits, but lacked detailed
21 analysis of the input system parameters and trade-offs.

22 Expanding the scope of our prior work (Chaudhari, Watkins et al. 2025), the novelty of the present
23 study is that we explore the environmental and socio-economic Pareto-front trade-offs, for the first
24 time, to depict the transition of recycling technologies in a circular economy along with their
25 relevant system-level metrics such as recycled content, circularity, and optimal need of virgin PET
26 (V-PET) resin. The study further strengthens the understanding of the system’s behavior such as
27 changes in material flows through each EOL process, inter-relationships between downstream
28 EOL and upstream processes, and changes in optimum selection of recycling technologies to
29 achieve a prescribed system performance (e.g. global warming potential (GWP), revenues, etc.)
30 via Pareto-front trade-off analysis and sensitivity analyses. Finally, a novel Pareto-optimal based
31 decision diagram was developed for the circular PET packaging system relative to the linear
32 economy to help quantify trade-offs in sustainability metrics (e.g. GWP versus Revenues).

33 Research objectives of the present study are to: 1) Identify the key processes contributing the most
34 to environmental and socio-economic impacts of the PET packaging supply chain processes in a
35 linear as well as circular economy, using previously developed model (Chaudhari, Watkins et al.
36 2025); 2) Conduct sensitivity analysis to identify the key input parameters that have the most
37 influence on optimal environmental and socio-economic impacts; 3) Analyze Pareto-frontier trade-
38 offs between environmental and socio-economic impacts of U.S. PET packaging material in a
39 circular economy.

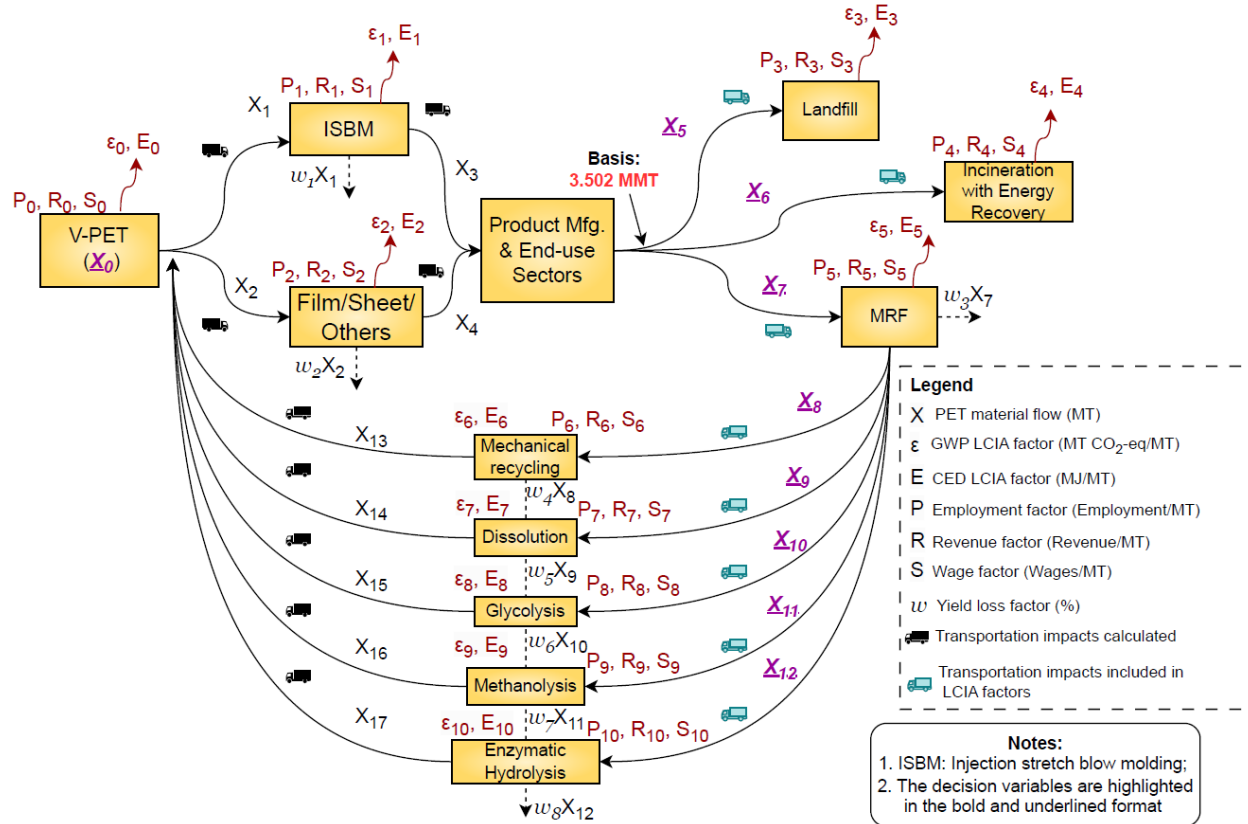
40 **2. METHODS**

1 Aligning with (Chaudhari, Watkins et al. 2025), material flow data was combined with
2 environmental life cycle impact assessment (LCIA) and socio-economic impact assessment factors
3 to optimize and evaluate sustainability impacts and trade-offs of PET packaging supply chains in
4 the U.S. The study considered two environmental indicators; global warming potential (GWP) and
5 cumulative energy demand (CED), that are frequently considered/reported (Zanghelini, Cherubini
6 and Soares 2018, Zhao, Walker et al. 2021) and used in decision making processes by organizations
7 (Subal, Braunschweig and Hellweg 2024). Furthermore, the study considered three socio-
8 economic indicators; employment, wages, and revenues, that are based on the North American
9 Industry Classification System (NAICS) codes used by U.S. Federal agencies for analyzing the
10 statistics related to the U.S. economy.

11 In addition to these indicators, systems level recycled content and circularity metrics for PET
12 material were also evaluated, which followed the definitions by (Di, Reck et al. 2021) and (Ellen
13 MacArthur Foundation 2019), respectively. The definitions and formulas for calculating material
14 circularity, recycled content, and the number of PET material use cycles in the system are shown
15 in Section S2.1 of the SI document. The following sections provide additional details on the system
16 analysis model, mathematical formulation and input data behind the optimization models, and
17 sensitivity analysis.

18 **2.1 System Analysis Model for PET Packaging Material**

19 The systems analysis model shown in Figure 1, adapted from (Chaudhari, Watkins et al. 2025),
20 aligns with our previously published systems analysis framework for plastics in a circular economy
21 (Shonnard, Tipaldo et al. 2019, Chaudhari, Lin et al. 2021). It involves the major existing and
22 emerging PET packaging material supply chain processes in the U.S., including transportation
23 steps to move material from one system process to another.



1
2 **Figure 1.** Simplified circular system analysis model for the PET packaging supply chain in the
3 U.S., adapted from (Chaudhari, Watkins et al. 2025). Notes: The environmental impacts of
4 delivering baled feedstock to glycolysis and methanolysis processing facilities via truck were
5 included in this work, which were missing in our prior work (Chaudhari, Watkins et al. 2025).
6 All of the environmental and socio-economic factors are material based, which are summarized
7 later in Section 2.3. MMT = Million metric tons.

8 Briefly, the U.S. PET packaging system includes following processes: 1) production of (V-PET
9 resin, mainly from non-renewable sources of feedstocks (i.e. crude oil and natural gas); 2) semi-
10 manufacturing processes such as injection stretch blow molding (ISBM), film/ sheet extrusion,
11 thermoforming processes for packaging applications only (Rosato, Rosato and v Rosato 2004,
12 Schott, Rosato and Rosato 2010); 3) EOL management processes such as collection, landfilling,
13 incineration with energy recovery, material recovery facility (MRF); 4) commercially practiced
14 mechanical recycling technology; and 5) emerging recycling technologies such as solvent-based
15 dissolution precipitation, glycolysis, methanolysis, and enzymatic hydrolysis processes. A
16 summary of each supply chain process aligning with Figure 1 is provided in Sections S2.2.1 to
17 S2.2.7 of the SI document.

18 The main output product produced from mechanical recycling and solvent-based dissolution-
19 precipitation recycling technologies are in the form of recycled PET (R-PET) resin. The difference
20 between these two is the quality of R-PET resin obtained from the processes. The emerging
21 solvent-based dissolution-precipitation recycling technology produces a high-quality recycled

1 resin that is comparable to fossil-derived resin (Xu, Sanchez-Rivera et al. 2025). Glycolysis,
2 methanolysis, and enzymatic hydrolysis processes can be categorized as “depolymerization”
3 recycling technologies (Ragaert, Ragot et al. 2023), that breaks the PET polymeric structure in the
4 presence of ethylene glycol, methanol, enzymes, respectively, to produce intermediate monomers
5 such as bis (2-hydroxyethyl) terephthalate (BHET) (from glycolysis), dimethyl terephthalate
6 (DMT) (from methanolysis), terephthalic acid (TPA) (from enzymatic hydrolysis) along with
7 ethylene glycol (Singh, Rorrer et al. 2021, Li, Aguirre-Villegas et al. 2022). These intermediate
8 monomers are then further polymerized to produce virgin quality R-PET resin (Garcia-Gutierrez,
9 Amadei et al. 2023). Therefore, the modeled depolymerization recycling technologies represent
10 “plastic-to-monomer-to-plastic” circular processes and impacts. Additionally, all of the recycling
11 technologies included the necessary bale pretreatment steps such as opening of bales, size
12 reduction to flakes, wet or dry sorting techniques, washing, and drying. Process yield loss at each
13 of these recycling steps is also included in the analysis, and is assumed to be landfilled and
14 incinerated, as described next.

15 The life cycle impacts of the pretreatment processes were inherently included as a part of the GWP
16 and CED LCIA factors for these emerging recycling technologies, which are summarized in the
17 following section. The total process waste generated (shown by dashed lines in Figure 1) was
18 assumed to be 80% landfilled and 20% incinerated with energy recovery consistent with
19 conventional disposal of waste plastics in the U.S. (U.S. EPA 2020). The transportation impacts
20 that are not included in the LCIA factors (see Figure 1 legend) were calculated separately as
21 described in our previous study, which assumed U.S. average transportation modes by truck
22 (54.8%), rail (34.1%), ocean (10.7%), and air (0.4%) (U.S. Department of Transportation Bureau
23 of Transportation Statistics 2021, Chaudhari, Johnson et al. 2022).

24 **2.2 Optimization Model Formulation**

25 Our study presents a material network flow multi-objective linear programming optimization
26 problem for the closed-loop PET packaging system shown in Figure 1. Aligning with (Chaudhari,
27 Watkins et al. 2025), the purpose of this optimization model is to determine environmentally and
28 socio-economically optimum EOL management of PET packaging waste in the U.S. Specifically,
29 the objective of this model is to minimize the environmental impacts and maximize the socio-
30 economic impacts of the entire PET packaging system (Figure 1) to determine environmentally
31 and socio-economically optimal EOL PET packaging material flows and relevant processes in the
32 system. As the study considered a total of five sustainability indicators, the system was optimized
33 individually on each of the sustainability indicators to generate a range of optimal solutions.

34 Following are the brief assumptions related to the optimization model. The total amount of PET
35 packaging waste generated (3.502 MMT) annually in the U.S. was assumed to be the material flow
36 basis (or starting point) for this static optimization model (Figure 1), which was based on (U.S.
37 EPA 2020) data (see SI section S2.2.3 for more information). As one of the research questions is
38 to determine how the PET packaging waste should be managed at the EOL, consumer behavior is
39 not taken into consideration but assumes 100% consumer participation in recycling. Hence, the
40 key material flow results from the optimization model can help inform the consumer to better

1 understand the environmental and socio-economic benefits and/or implications of EOL waste
2 management.

3 As the packaging products have a very short in-use lifetime of less than one year, we assumed zero
4 accumulation of PET packaging material in the system (i.e. no material in “use” stocks and the
5 total PET material converted into packaging products is equal to the total PET packaging waste
6 generated). Furthermore, mismanagement or leakages of PET material to land and ocean
7 ecosystems were excluded considering well-established EOL recycling infrastructure in the U.S.
8 (Jambeck, Geyer et al. 2015). The PET packaging waste can be collected via curbside collection
9 programs and/or bottle deposit programs for PET bottles only (Chaudhari, Johnson et al. 2022,
10 Smith, Takkellapati and Riegerix 2022). The present study excluded optimization/modelling of
11 material flows through bottle deposit programs to simplify the model as well as due to limited
12 availability of the socio-economic data for bottle deposit programs. The optimization model was
13 solved using the Simplex Linear Programming (LP) Excel Solver.

14 From an environmental perspective, the system was optimized by minimizing annual GWP
15 (millions of metric tons (MMT) CO₂-eq; equation (1)) and CED (PJ; equation (2)) of the entire
16 system (Figure 1). From a socio-economic perspective, the system was optimized by maximizing
17 employment (employees; equation (3)), revenues (\$billion; equation (4)), and wages (\$billion;
18 equation (5)) of the entire system. The environmental and socio-economical objective functions
19 are mathematically expressed as follows:

$$\begin{aligned} \text{Min. GWP: } & \varepsilon_0 X_0 + \varepsilon_1 X_3 + \varepsilon_2 X_4 + \varepsilon_3 X_5 + \varepsilon_4 X_6 + \varepsilon_5 (X_8 + X_{10} + X_{11} + X_{12}) + \varepsilon_6 X_{13} + \varepsilon_7 X_{14} \\ & + \varepsilon_8 X_{15} + \varepsilon_9 X_{16} + \varepsilon_{10} X_{17} \\ & + \varepsilon_3 (0.8 \times (w_1 X_1 + w_2 X_2 + w_3 X_7 + w_4 X_8 + w_6 X_{10} + w_7 X_{11} + w_8 X_{12})) \\ & + \varepsilon_4 (0.2 \times (w_1 X_1 + w_2 X_2 + w_3 X_7 + w_4 X_8 + w_6 X_{10} + w_7 X_{11} + w_8 X_{12})) \end{aligned} \quad (1)$$

$$\begin{aligned} \text{Min. CED: } & E_0 X_0 + E_1 X_3 + E_2 X_4 + E_3 X_5 + E_4 X_6 + E_5 (X_8 + X_{10} + X_{11} + X_{12}) + E_6 X_{13} + E_7 X_{14} \\ & + E_8 X_{15} + E_9 X_{16} + E_{10} X_{17} \\ & + E_3 (0.8 \times (w_1 X_1 + w_2 X_2 + w_3 X_7 + w_4 X_8 + w_6 X_{10} + w_7 X_{11} + w_8 X_{12})) \\ & + E_4 (0.2 \times (w_1 X_1 + w_2 X_2 + w_3 X_7 + w_4 X_8 + w_6 X_{10} + w_7 X_{11} + w_8 X_{12})) \end{aligned} \quad (2)$$

$$\begin{aligned} \text{Max. Emp.: } & P_0 X_0 + P_1 X_1 + P_2 X_2 + P_3 X_5 + P_4 X_6 + P_5 X_7 + P_6 X_8 + P_7 X_9 + P_8 X_{10} + P_9 X_{11} \\ & + P_{10} X_{12} \\ & + P_3 (0.8 \times (w_1 X_1 + w_2 X_2 + w_3 X_7 + w_4 X_8 + w_5 X_9 + w_6 X_{10} + w_7 X_{11} \\ & + w_8 X_{12})) \\ & + P_4 (0.2 \times (w_1 X_1 + w_2 X_2 + w_3 X_7 + w_4 X_8 + w_5 X_9 + w_6 X_{10} + w_7 X_{11} \\ & + w_8 X_{12})) \end{aligned} \quad (3)$$

$$\begin{aligned} \text{Max. Rev.: } & R_0 X_0 + R_1 X_1 + R_2 X_2 + R_3 X_5 + R_4 X_6 + R_5 X_7 + R_6 X_8 + R_7 X_9 + R_8 X_{10} + R_9 X_{11} \\ & + R_{10} X_{12} \\ & + R_3 (0.8 \times (w_1 X_1 + w_2 X_2 + w_3 X_7 + w_4 X_8 + w_5 X_9 + w_6 X_{10} + w_7 X_{11} \\ & + w_8 X_{12})) \\ & + R_4 (0.2 \times (w_1 X_1 + w_2 X_2 + w_3 X_7 + w_4 X_8 + w_5 X_9 + w_6 X_{10} + w_7 X_{11} \\ & + w_8 X_{12})) \end{aligned} \quad (4)$$

$$\begin{aligned}
\text{Max. Wage: } & S_0X_0 + S_1X_1 + S_2X_2 + S_3X_5 + S_4X_6 + S_5X_7 + S_6X_8 + S_7X_9 + S_8X_{10} + S_9X_{11} \\
& + S_{10}X_{12} \\
& + S_3 (0.8 \times (w_1X_1 + w_2X_2 + w_3X_7 + w_4X_8 + w_5X_9 + w_6X_{10} + w_7X_{11} \\
& + w_8X_{12})) \\
& + S_4 (0.2 \times (w_1X_1 + w_2X_2 + w_3X_7 + w_4X_8 + w_5X_9 + w_6X_{10} + w_7X_{11} \\
& + w_8X_{12}))
\end{aligned} \tag{5}$$

1 For the symbols used in these equations, please refer to Figure 1. The decision variables of this
2 optimization are the material flows at the EOL (X_5 - X_{12}), and the amount of virgin PET (V-PET
3 (X_0)) required in the system (bolded, underlined and shown in violet color in Figure 1). Based on
4 the environmental, socio-economic, and process yield loss factors, the model will predict whether
5 to process this waste for disposal (i.e. landfill or incineration) or for recycling through MRF, and
6 if so, through which type(s) of recycling technology. The output recycled resin material flows (X_{13} -
7 X_{17}) from optimally selected recycling technologies would further be blended with V-PET resin
8 for manufacturing of semi-finished packaging products.

9 All these objective functions were subjected to mass balance constraints at each supply chain stage
10 (constraints no. 1 to 8) and an additional technical constraint on the mechanically recycled resin
11 (constraint no. 9), as shown in Table 2. A maximum blend limit of 35% was imposed only on the
12 mechanically recycled PET resin (Benavides, Dunn et al. 2018, Lange, Kersten et al. 2024) due to
13 the loss of quality and discoloration effects (Berg, Schaefer et al. 2016). The R-PET resin obtained
14 via other emerging recycling technologies is understood to be of near-fossil quality resin (Walker,
15 Frelka et al. 2020, Sánchez-Rivera, Zhou et al. 2021, Garcia-Gutierrez, Amadei et al. 2023).

16

17 **Table 2.** Summary of constraints used in the optimization model. Note: Please refer to Figure 1
18 for the symbols shown in these constraints.

Constraint No.	Constraint Description	Constraint Equation
1	Mass balance at EOL	$X_3 + X_4 = X_5 + X_6 + X_7$
2	Mass balance at MRF	$X_7 = X_8 + X_9 + X_{10} + X_{11} + X_{12} + w_3 X_7$
3	Mass balance at mechanical recycling	$X_8 = X_{13} + w_4 X_8$
4	Mass balance at dissolution	$X_9 = X_{14} + w_5 X_9$
5	Mass balance at glycolysis	$X_{10} = X_{15} + w_6 X_{10}$
6	Mass balance at methanolysis	$X_{11} = X_{16} + w_7 X_{11}$
7	Mass balance at enzymatic hydrolysis.	$X_{12} = X_{17} + w_8 X_{12}$

8	Mass balance between converters, and virgin and recycled plastic resins ("Demand" constraint)	$X_1 + X_2 = X_0 + X_{13} + X_{14} + X_{15} + X_{16} + X_{17}$
9	35% blend limit constraint on mechanically recycled resin	$X_{13} \leq 0.54 (X_0 + X_{14} + X_{15} + X_{16} + X_{17})$

1

2 **2.3 Overview of the Input Data**

3 The material-based LCIA factors, socio-economic impacts factors, and process yield loss factors
4 were gathered from the literature and are briefly summarized in Table 3 along with their respective
5 system boundaries shown below the table. As shown in Section 2.2 (objective function equations),
6 the total environmental and socio-economic impacts of the system were estimated by multiplying
7 material flows with respective environmental, socio-economic, and process yield loss factors,
8 considering the input or output mass basis and the system boundary of these factors.

9 The GWP LCIA factors (MT CO₂-eq/MT) were gathered from the literature and are the key
10 outputs/results from the Intergovernmental Panel on Climate Change (IPCC) 2013 and/or 2021
11 GWP over a 100-year period life cycle impact assessment method, depending on the referenced
12 literature. Therefore, these factors for the PET supply chain processes include the contribution
13 from all greenhouse gases. The CED LCIA factors (MJ/kg) were also gathered from literature and
14 are the key output/results from the Cumulative Energy Demand (CED) life cycle impact
15 assessment method. The process-level GWP and CED LCIA factors were carefully reviewed to
16 ensure that the sourced/original studies followed the International Standards Organization (ISO)
17 standards for LCA and clearly stated their system boundaries, functional unit, and assumptions.
18 Additional process-level details, including system boundaries, are provided in Section S2.2.1-
19 S2.2.7 of the SI document.

20 Briefly, the “cradle-to-gate” LCIA factors for V-PET resin production and for mechanical recycling
21 processes, including collection, sorting at MRF, transportation to reclaimer, and reclaimer
22 operations to produce recycled PET resin, were obtained from Franklin Associates Reports
23 (Franklin Associates 2018, Franklin Associates 2020). The “gate-to-gate” LCIA factors for semi-
24 manufacturing processes were based on the Ecoinvent data (Wernet, Bauer et al. 2016) obtained
25 from the SimaPro v9.0, previously summarized in our work by (Chaudhari, Johnson et al. 2022).
26 The electricity grid mix for these semi-manufacturing processes was updated to reflect 2020 U.S.
27 average grid mix (U.S. Energy Information Administration (EIA) 2021). The “cradle-to-gate”
28 LCIA factors for landfilling and incineration with energy recovery were obtained from the U.S.
29 EPA WARM reports (U.S. EPA 2020). The LCIA factors for glycolysis and methanolysis were
30 based on (Uekert, Singh et al. 2023), that for enzymatic hydrolysis on (Gracida-Alvarez, Xu et al.
31 2023), and for solvent-based dissolution with precipitation via cooling approach was based on
32 (Chaudhari, Kulas et al. 2023). To account for the missing transportation impacts in the LCIA
33 factors for glycolysis and methanolysis reported by (Uekert, Singh et al. 2023), we assumed an
34 average baled feedstock transportation distance of 295 km via truck, based on (Gracida-Alvarez,
35 Xu et al. 2023). The GWP and CED LCIA factors used in this study for dissolution-precipitation

1 process are approximately 1% higher than (Chaudhari, Watkins et al. 2025) due to increased
 2 average baled transportation distance of 185 km via truck. The LCIA factors utilized in our system
 3 were attributional factors (i.e. no system expansion or credits due to avoided fossil feedstocks),
 4 except for the incineration with energy recovery, which was a consequential LCIA factor.

5 **Table 3.** Environmental LCIA and socio-economic indicators per metric ton (MT) of product or
 6 process throughput across the U.S. PET supply chain processes, adapted from (Chaudhari,
 7 Watkins et al. 2025).

PET Packaging Supply Chain Process	GWP LCIA Factors (MT CO ₂ -eq/MT)	CED LCIA Factors (MJ/kg)	Employment per MT	Revenue per MT (\$/MT) ^μ	Wages per MT (\$/MT) ^μ	Yield loss (%)
V-PET ^a	2.23	61.4	0.0017 ^μ	3,327.1	191.4	-
ISBM ^b	1.16	27.8	0.011 ^α	4,038.5	660.0	2.2
Film/Sheet/Others ^b	0.35	8.87	0.011 ^α	1,684.3	748.0	1.6
Landfill ^a	0.022	0.31	0.00073 ^α	212.5	46.8	-
Incineration with energy recovery ^{a, ‡}	1.37	-11.62	0.00073 ^α	201.0	44.4	-
Collection for recycling ^b	-	-	0.0016 ^α	505.6	112.0	-
MRF [†]	0.066	0.960	0.0017 ^β	637.5	91.8	11
Mechanical recycling ^b	0.838	13.61	0.003 ^δ	1,416.7	162.0	20
Dissolution-precipitation ^{a, *}	1.09	18.05	0.003 ^δ	1,441.4	317.7	11
Glycolysis ^b	1.36	29.37	0.006 ^δ	1,290.3	635.4	24
Methanolysis ^b	4.23	73.07	0.006 ^δ	1,290.3	635.4	24
Enzymatic hydrolysis ^b	3.25	57	0.006 ^δ	1,221.4	635.4	31

8 *Notes: ‘a’: “cradle-to-gate” system boundary; ‘b’: “gate-to-gate” system boundary; ‘‡’: Includes environmental credits for displaced electricity from fossil feedstocks; ‘†’: environmental impacts are “cradle-to-gate” (includes collection and sorting at MRF), whereas socio-economic impacts are “gate-to-gate”; ‘*’: Includes the environmental impacts of collection, sorting at MRF, transportation, and process specific impacts, whereas socio-economic impacts are “gate-to-gate”; ‘μ’: Authors’ estimate based on NAICS codes; ‘α’: (Goldstein and Electris 2011); ‘β’: (Hestin, Faninger and Milios 2015); ‘δ’: (Nordic Council of Ministers; Systemiq 2023); All LCIA factors were on an output mass basis, except for landfill and incineration with energy recovery, which is on an input mass basis. The socio-economic factors were on an input mass basis, except for virgin PET, which is on an output basis.*

18 The employment per metric ton (MT) factors were gathered from the literature (see information
 19 below Table 3), except for the V-PET resin production, which was estimated by combining material
 20 flow data, life cycle inventory data, and industry sector data based on NAICS codes (IBIS World
 21 2023, Chaudhari, Sedaghatnia et al. 2024). The socio-economic factors for V-PET resin production
 22 represent a “cradle-to-gate” system boundary, including the extraction and processing of crude oil

1 and natural gas to production of the final PET resin. The revenues and wages per MT factors were
2 estimated based on the employment per MT factors using the revenues per employee and wages
3 per employee factors, respectively, obtained from the industry specific NAICS codes (IBIS World
4 2023), with an exception for the revenues per MT factors for recycling technologies. The revenue
5 per MT factor for mechanical recycling was assumed to be the 10-year average market price of
6 mechanically recycled PET resin, which is \$1,700/MT. The revenues per MT factors for all other
7 emerging recycling technologies were assumed to be equal to the 10-year average price of virgin
8 PET resin, which is \$1,600/MT. These revenue/MT factors were converted to a process input basis
9 using process yield loss factors. The socio-economic data for these emerging recycling
10 technologies are limited and not well understood to know which industrial sector codes they would
11 belong to. We recognize this limitation of the present study and subject these input parameters for
12 the sensitivity analysis.

13 **2.4 Pareto Front Trade-off Analysis: Epsilon (ϵ)-Constraint Method**

14 The Pareto front analysis helps the decision makers to gain additional insights about alternative
15 optimal system designs and quantitatively identify the trade-offs among different objectives (Wang
16 and Rangaiah 2017). Particularly, it can help decision makers to quantify and depict the changes
17 in material flows across the system processes, including the transition of recycling technologies,
18 and help understand the inter-relationships among the system metrics and material flows. A Pareto
19 front analysis generates a set of non-dominated solutions (or Pareto optimal solutions), wherein
20 one objective function cannot be improved without hurting at least one of the other objective
21 functions (Azapagic and Clift 1999, Cohon 2004, Mavrotas 2009, Gunantara 2018). The choice of
22 selecting from the Pareto optimal solutions would ultimately be dictated by the decision maker's
23 preferences and willingness to trade off one objective for the others (Azapagic and Clift 1999,
24 Mavrotas 2009). Selection of an alternative system design among Pareto optimal solutions requires
25 use of additional multi-criteria decision-making methods (Cabo 2024) and is out of scope for the
26 present study.

27 The present study utilized one of the most widely used (Branke 2008, Sandoval-Reyes, He et al.
28 2024) and well-established (Heidari, Yazdanparast and Jabbarzadeh 2019) ϵ -constraint (epsilon
29 constraint) methods to solve the multi-objective linear programming optimization problem, which
30 was previously introduced by (Haimes 1971). In our study, this method is used to generate a set of
31 alternative Pareto optimal solutions between conflicting environmental and socio-economic
32 objectives. In ϵ -constraint method, a primary objective function is selected to be optimized while
33 constraining other remaining objective functions to a certain epsilon (ϵ) value along with an initial
34 set of regular constraints (i.e. in our case the mass balance and blend limit constraints, shown in
35 Table 2) (Azapagic and Clift 1999, Cohon 2004, Mavrotas 2009). The ϵ -values of the constrained
36 objective functions are then varied systematically to generate Pareto optimal solutions (Azapagic
37 and Clift 1999). These ϵ -values are obtained from the range of optimal values observed from the
38 single optimization run, as mentioned in the above Section 2.2 ('Optimization Model
39 Formulation'). A brief summary of the steps involved in the ϵ -constraint method is provided by
40 (Azapagic and Clift 1999, Cohon 2004).

1 In our study, minimizing GWP was chosen as a primary objective function from an environmental
2 perspective. A Pareto front analysis was conducted between GWP and other socio-economic
3 indicators. A simplified overall approach to conducting this analysis can be summarized as follows:

4 *Minimize* GWP (From above equation no. 1)

5 *Subject to*

6 Mass balance constraints (From above constraint nos. 1-8)

7 Blend limit constraint (From above constraint no. 9)

8 Revenue Constraint (From above equation no. 4) $\geq \epsilon_{\text{Revenue}}$

9 Employment Constraint (From above equation no. 3) $\geq \epsilon_{\text{Employment}}$

10 Wage Constraint (From above equation no. 5) $\geq \epsilon_{\text{Wage}}$

11 CED Constraint (From above equation no. 2) $\leq \epsilon_{\text{CED}}$

12 The $\epsilon_{\text{Revenue}}$, $\epsilon_{\text{Employment}}$, ϵ_{Wage} , and ϵ_{CED} on the right hand side (RHS) of the constraints represent
13 the epsilon values showing the minimum value of revenue, employment, wage, and the maximum
14 value of CED, respectively, identified based on individual optimization runs. For example, to
15 evaluate the trade-offs between GWP and revenues, the $\epsilon_{\text{Revenue}}$ would be systematically varied
16 between the identified range (based on single optimization runs) and the model would be solved
17 again to minimize the GWP of the system for a given $\epsilon_{\text{Revenue}}$ without violating any of the
18 constraints mentioned above.

19 **2.5 Sensitivity Analysis**

20 A sensitivity analysis was performed on some of the key input parameters to the system
21 optimization models. The purpose of this analysis is to understand the system behavior due to a
22 change in key input parameters on the selection of EOL recycling technologies by the optimization
23 model and the relative change in system performance metrics. These input parameters included
24 LCIA factors, socio-economic, process yield loss factors, and the blend limit constraint on
25 mechanically recycled resin. These parameters were varied one at a time by +30% (high scenario)
26 and -30% (low scenario) and the optimization model was solved again to understand their effect
27 on the optimal solutions (e.g. min. GWP, min. CED, max. revenues, max. employment, and max.
28 wages), while monitoring the changes on the other system indicators.

30 **3. RESULTS AND DISCUSSION**

31 **3.1 Optimal Circular PET Packaging System: Pay-off Table**

32 A summary of optimization results is displayed in Table S1 in the form of a pay-off table. This
33 pay-off table helps to understand initial information such as the range of optimal solutions for each
34 objective function along with relevant system-level sustainability metrics, selected decision
35 variables, and simple overview of trade-offs among analyzed metrics. The optimization results in

1 the form of material flow Sankey diagram are previously discussed and presented in our prior work
2 (Chaudhari, Watkins et al. 2025). The updated LCIA factors for glycolysis, methanolysis, and
3 dissolution processes (see Figure 1 caption and section 2.3) resulted in a difference of less than
4 1% between the optimal values of GWP and CED (Table S1), compared to those in (Chaudhari,
5 Watkins et al. 2025). Following is a brief summary of the optimization results.

6 To minimize environmental impacts and maximize socio-economic impacts, the optimization
7 model predicted a true circular economy showing 100% collection rate for recycling of PET
8 packaging waste ($X_7 = 3.502$ MMT) with zero percent disposal rate ($X_5 = X_6 = 0$ MMT). After
9 collecting and sorting through MRFs, the model optimally predicted solvent-based dissolution-
10 precipitation recycling technology when optimized on minimizing environmental impacts (i.e.
11 from environmental perspective). On the other hand, enzymatic hydrolysis recycling technology
12 was selected when optimized on maximizing socio-economic impacts (i.e. from socio-economic
13 perspective). A maximum circularity of 77% (see Table S1) was achieved when optimizing from
14 an environmental perspective, producing a total of 2.774 MMT of high-quality recycled resins
15 with a need/requirement of 0.803 MMT of V-PET resin into the system. The environmentally
16 optimal system showed 78% reduction in the demand for V-PET resin, compared to V-PET demand
17 in linear economy. On the other hand, a maximum circularity of 59% (see Table S1) was achieved
18 when optimizing from a socio-economic perspective producing a total of 2.151 MMT of high-
19 quality recycled resins with an optimal need of 1.426 MMT of V-PET resins into the system. This
20 represents 60 % reduction in the demand for V-PET resin, compared to that in linear economy.

21 The optimization model resulted in a closure of mass balance around all the processing steps,
22 including the demand constraint (see Table 2). Moreover, the total mass of V-PET resin was found
23 to be equal to the total mass of PET material disposed to landfills and incineration with energy
24 recovery processes. This finding further implies that V-PET material is only needed to make up
25 for the material lost as waste during all the processing steps (semi-manufacturing, MRFs, recycling
26 technologies) as well as to meet the demand for the semi-manufacturing processes.

27 Minimizing the environmental impacts of PET packaging system led to selection of dissolution-
28 precipitation technology due to the higher process yield (i.e. lower generation of process waste to
29 be managed via disposal processes), which ultimately requires a lesser amount of emission- and
30 energy-intense V-PET resin entering into the system. Lowering the loss of PET material to landfills
31 or incineration due to waste prevention measures at each of the system processes means lowering
32 the need for emissions-and-energy intense V-PET resin that needs to be balanced to meet the
33 demand for semi-manufacturing processes. Maximizing the socio-economic impacts of the PET
34 packaging system avoided disposal processes (i.e. landfilling and incineration) due to their low
35 socio-economic benefits (revenues, wages, employment) as compared to recycling processes.

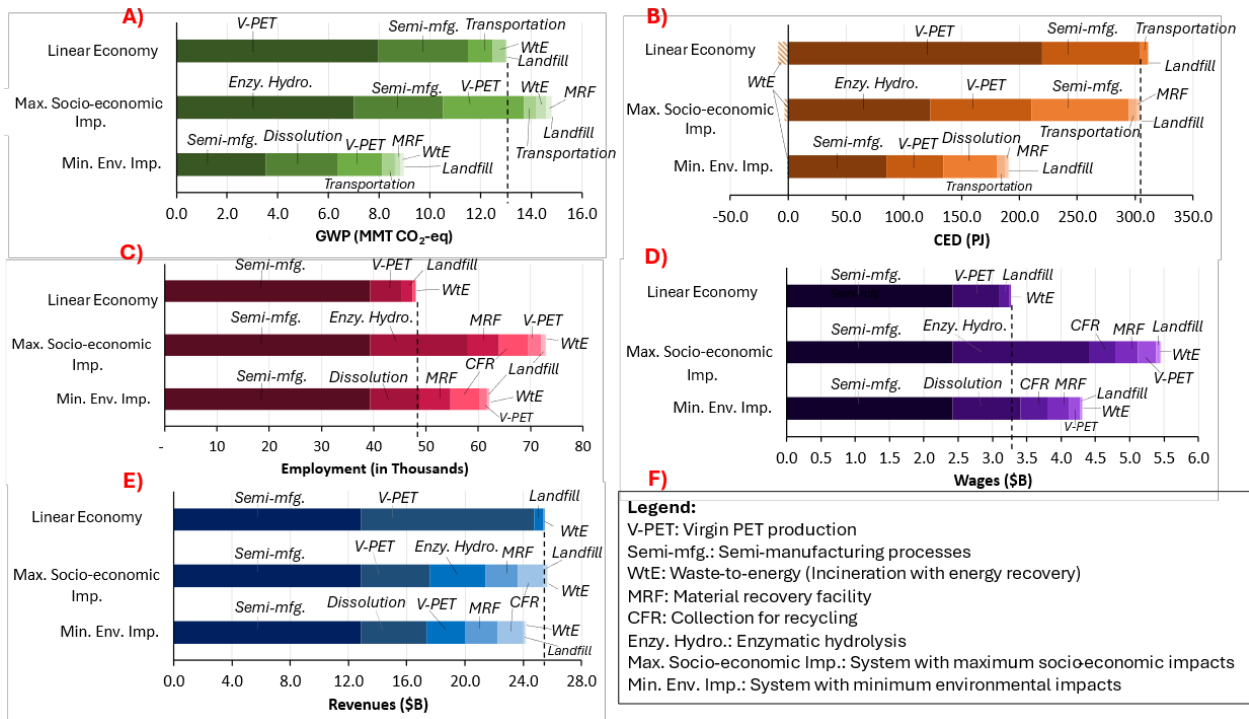
36 Table S1 also shows that optimizing either of the environmental indicators resulted in the same
37 results/system configuration i.e. 100% collection for recycling of PET packaging waste at EOL,
38 followed by recycling via solvent-based dissolution-precipitation technology. Similar findings can
39 be observed for the system optimized on socio-economic indicators but with a different selection
40 of recycling technology, which in this case was enzymatic hydrolysis. Prior work by (Azapagic
41 and Clift 1999) reported similar finding for multi-objective optimization of boron product system

1 that optimizing on any one of the environmental objective functions optimizes all other
 2 environmental impacts. However, this finding may not be always true as the optimal results depend
 3 on the system configuration itself as well as the input data to the system model.

4 Overall, a trade-off between environmental and socio-economic metrics can be observed from
 5 Table S1. For example, the environmentally optimum system resulted in a much lower system
 6 GWP and CED when compared to the socio-economic optimum system. However, the
 7 environmentally optimal system exhibited lower employment (by 15%), lower revenues (by 6%),
 8 and lower wages (by 21%), when compared with socio-economically optimal system. Moreover,
 9 optimizing the socio-economic impacts led to reduced circularity and recycled content compared
 10 to the environmentally optimal system, which was mainly due to higher loss of PET material as
 11 process waste to landfills and incineration during all the processing steps. Finally, the pay-off table
 12 also forms a basis for the ϵ -constraint method by identifying the minimum and maximum values
 13 of the epsilon (ϵ): revenue (\$24.19-\$25.71 billion), employment (62,200-73,065), wages (\$4.31 -
 14 \$5.45 billion), and CED (189.72-301.49 PJ).

15 3.2 Linear and Optimal Circular PET Packaging Systems

16 Figure 2 shows a comparison of sustainability impacts of environmentally and socio-economically
 17 optimum systems with the linear PET packaging system. Furthermore, these impacts are also
 18 broken down by PET packaging supply chain processes. The linear PET packaging system is only
 19 a scenario (i.e. no optimization) representing 80% of the waste PET being landfilled, 20%
 20 incinerated with energy recovery (or waste-to-energy (WtE)), and no (i.e. zero) recycling at the
 21 EOL.



1 **Figure 2.** Environmental and socio-economic impacts at a process level in linear and optimal
2 circular PET packaging systems. Notes: The dashed vertical line on each graph represents the
3 total or net impact of linear economy system, which serves as the reference point against the two
4 other optimum systems.

5 In the linear PET packaging system ('Linear Economy'), the environmental impacts (Figure 2 A-
6 B) are mainly dominated by the fossil-derived V-PET resin, whereas the socio-economic impacts
7 (Figure 2 C-E) are dominated by the semi-manufacturing processes. In optimal circular PET
8 packaging systems, all these impacts were mainly dominated by semi-manufacturing processes
9 and/or optimally selected recycling technology processes with the least contributions from
10 traditional disposal processes (e.g. landfill and WtE). Overall, the shift from a linear to an optimum
11 closed-loop circular economy of PET packaging systems showed a shift from fossil-based
12 traditional technologies to emerging recycling technologies resulting in higher employment,
13 wages, recycled content, and system circularity. The next subsections show environmental (section
14 3.2.1) and socio-economic (section 3.2.2) performance comparison of optimal systems with linear
15 systems.

16 **3.2.1 Environmental Performance Compared to Linear PET Packaging System**

17 The total GWP and net CED impacts of the linear system were found to be 13.03 MMT CO_{2-eq} and
18 303.5 Petajoules (PJ), respectively (Figure 2 A-B). The environmentally optimum system resulted
19 in GWP and CED savings of 31% and 37%, respectively, compared to the linear PET packaging
20 system (Figure 2 A-B).

21 For the environmentally optimum system, the semi-manufacturing processes have the highest
22 material flow throughput that contributed the most (39%) to the total systems GWP, followed by
23 dissolution (31%), V-PET resin production (20%), transportation (6%), MRF operations (2%),
24 incineration with energy recovery (1%), and landfill (<0.1%). In terms of the CED of the
25 environmental optimum system, V-PET resin production which had a relatively small magnitude
26 of material flow (0.803 MMT), contributed the most (26%) after semi-manufacturing processes
27 (45%).

28 The environmental impacts of socio-economically optimum PET packaging system resulted in
29 14% higher GWP but less than 1 % savings of CED compared to the linear system (Figure 2 A-
30 B). The optimization model selected enzymatic hydrolysis process to recycle PET to maximize the
31 socio-economic impacts of the system, which is associated with higher GWP and lower CED than
32 production of V-PET resin (see Table 3). Therefore, most of these total environmental impacts
33 were dominated by the enzymatic hydrolysis process.

34 **3.2.2 Socio-economic Performance Compared to Linear PET Packaging System**

35 The employment, wages, and revenues of the linear PET packaging system were found to be
36 48,034 employees (Figure 2C), \$3.27 billion (Figure 2D), and \$25.50 billion (Figure 2E),
37 respectively. All these impacts were mainly dominated by the semi-manufacturing and V-PET resin
38 production processes. The contribution of linear/disposal EOL processes to the total employment,
39 wages, and revenues of the linear PET packaging system were found to be 5%, 3%, and 5%,

1 respectively. This further means that manufacturing processes contribute more to the overall socio-
2 economic impacts of the system than disposal of waste PET to landfill and incineration processes
3 (*WtE*).

4 The employment and wages of environmentally circular PET packaging system were 29% and
5 32% higher, respectively, than the linear system. Most of these employment and wages in
6 environmentally optimal systems are dominated by semi-manufacturing processes and recycling
7 processes, including dissolution-precipitation technology. However, the environmentally circular
8 system showed a loss in revenue of 5% compared to the linear system. Overall, the
9 environmentally optimum system has higher environmental and social benefits compared to the
10 linear PET packaging system, except for a loss in revenues of 5%. This loss in revenue was mainly
11 due to the reduced amounts of virgin PET resin, which is associated with higher revenues than
12 recycled resins.

13 The employment, wages, and revenues of the socio-economically optimum system were 52%,
14 67%, and 1% higher than that of linear PET packaging system. However, all these socio-economic
15 benefits also came at a cost of increased GWP by 14% and less than 1% savings of CED than the
16 linear PET packaging system. Overall, the socio-economically optimum system exhibited higher
17 environmental impacts or closer to the linear system impacts but resulted in the most significant
18 gains in employment and wages for a small increase in the revenues, compared to the linear
19 economy.

20 **3.3. SENSITIVITY ANALYSIS**

21 The sensitivity analysis results for the U.S. PET packaging system optimized on GWP are shown
22 in Figure 3A-F. The key input parameters affecting the optimal GWP were found to be the GWP
23 LCIA factors for the following processes: dissolution-precipitation, production of V-PET resin,
24 mechanical recycling, and process yield loss factors for dissolution-precipitation, MRF, and
25 mechanical recycling processes.

26 An increase or decrease in any of the other listed parameters did not significantly affect either the
27 optimal GWP value or other system metrics. Overall, $\pm 30\%$ change in the above-mentioned
28 parameters, except for the MRF yield loss, showed 100% EOL recycling of all PET packaging
29 material with a combination of mechanical recycling (maximized up to the blend limit of 35%)
30 and dissolution-precipitation recycling processes, indicated by the star shown in Figure 3.

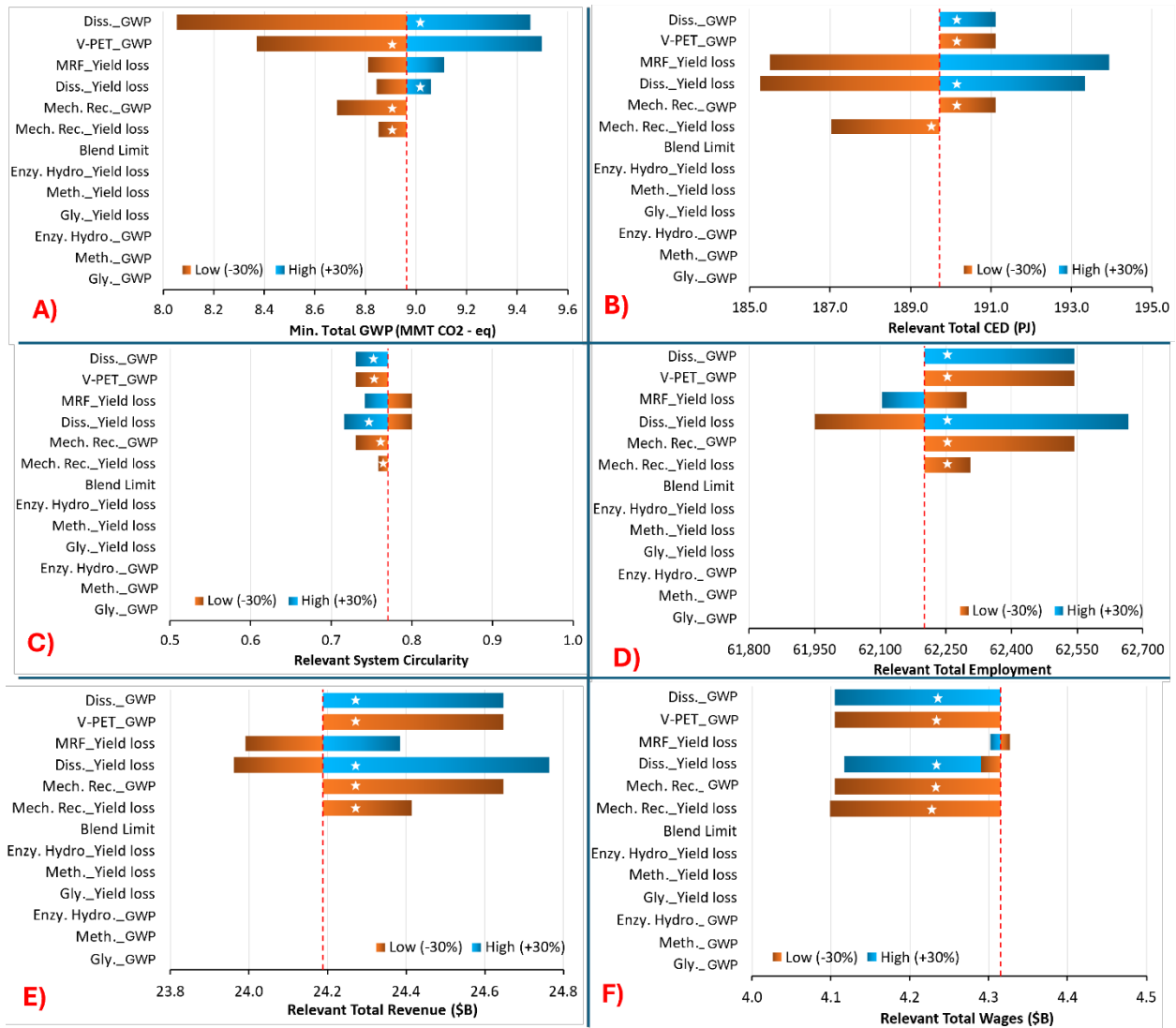


Figure 3. Sensitivity analysis results for the PET packaging system optimized for minimizing GWP. Note: The bars marked with a white star indicate a change in the optimal solution (or decision variables such as X_5 - X_{12} , X_0) predicted by the optimization model; Absence of white star indicates no change in the optimal solution. Figure 3A: Optimal GWP value; Figure 3B-F: Relevant values of system metrics such as CED, circularity, employment, revenues, and wages, respectively. The red dashed line represents the relevant optimal values when system is minimized for GWP.

A 30% decrease (“low scenario”; orange color) in the GWP LCIA factor for dissolution-precipitation process led to a 10% decrease in the optimal GWP value without changing the optimal decision variables at the EOL. However, a 30% increase (“high scenario”; blue color) for this same parameter led to a 5% increase in the GWP *with a* change in optimal solution (as indicated by star in Figure 3A) to be a combination of maximized mechanical recycling (i.e. up to the blend limit constraint) and dissolution-precipitation recycling processes, whereas in Figure 2A, only dissolution-precipitation is selected at EOL as optimum.

1 The resulting changes due to one parameter on other system metrics are shown in Figure 3 B-F.
2 For example, a 30% increase in the GWP LCIA factor for dissolution-precipitation process led to
3 increased CED (by 0.7%), reduced system circularity (by 5%), increased employment (by 0.6%)
4 and revenues (by 2%), and decreased wages (by 5%), compared to their respective base values.
5 These increased or decreased system metrics are a result of the combination of these two recycling
6 technologies, which lead to more generation of process waste requiring more use of V-PET into
7 the system. It is interesting to note here that increasing GWP LCIA factor for dissolution process
8 by 30% led to 5 % decrease in wages (Figure 3F). This was mainly due to lower wages associated
9 with mechanical recycling (selected up to the blend limit), compared to dissolution-precipitation.
10 The results of sensitivity analysis on optimal solutions of CED, employment, wages, and revenues
11 are presented in Figure S1-S4, respectively, in the SI document (Section S4).

12 **3.4. Environmental and Socio-economic Trade-offs**

13 **3.4.1 Pareto frontier between GWP and revenues**

14 Figure 4 shows the results of Pareto front analysis between total GWP (primary Y-axis; blue color)
15 and revenues (X-axis) of the PET packaging system. The results shown in Figure 4 represent an
16 analysis of the system that is optimized on minimizing GWP subject to constraints on mass
17 balance, blend limit, revenues, employment, wages, and energy of the system, as mentioned in
18 section 2.4. The RHS epsilon value of revenue was systematically varied between the identified
19 range shown in Table S1. The model was solved for each varied epsilon while simultaneously
20 noting the key results and system metrics from the optimization runs. The values of $\epsilon_{\text{Employment}}$, ϵ_{Wage} ,
21 and ϵ_{CED} on the RHS of employment, wages, and CED constraints were 62,200 employment,
22 \$4.31 billion, and 301.49 PJ, respectively.

23 Briefly, Figure 4 shows a set of alternative Pareto optimal solutions or a set of alternative PET
24 packaging system designs (shown by colored boxes) between the environmentally (red star) and
25 socio-economically (black star) optimal systems. Additionally, Figure 4 also depicts other system
26 metrics observed from the Pareto optimal solutions on the secondary (right) Y-axis in orange color
27 (wages in Figure 4A; employment in Figure 4B; system circularity in Figure 4C; V-PET in system
28 in Figure 4D). Moreover, Figure 4E shows the relevant EOL management of PET packaging
29 material, and Figure 4F shows the combinations/transition of EOL recycling technologies due from
30 the Pareto front analysis. The percentages shown in Figure 4E are based on the total PET packaging
31 waste generated at the EOL (i.e. X_5 , X_6 , and X_7 from Figure 1). The percentages shown in Figure
32 4F are based on the total baled PET shipped from MRF (i.e. X_8 to X_{12} from Figure 1) to different
33 recycling technologies.

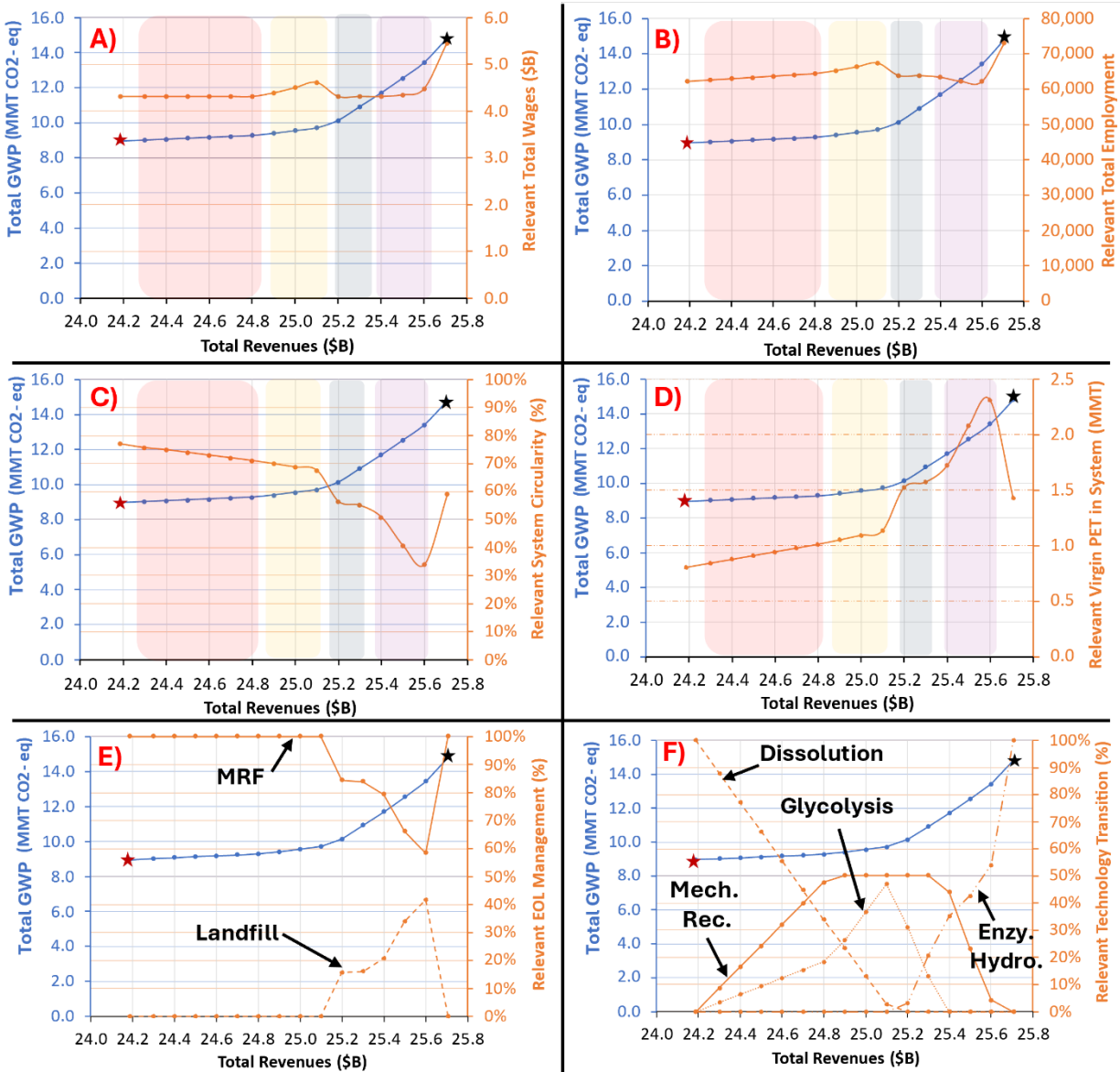
34 Overall, these results show that a 6% increase in the revenues of the system increased the total
35 GWP by 65% from environmentally optimum to socio-economically optimum PET packaging
36 systems. Depolymerization recycling technologies (e.g. glycolysis, enzymatic hydrolysis) are
37 needed to balance for the lower socio-economic impacts associated with mechanical recycling and
38 dissolution-precipitation recycling technologies with a transition from environmental to socio-
39 economic optimal systems (over the range of $\epsilon_{\text{Revenue}}$). Moreover, a reduced circularity of the PET
40 packaging system was also observed with a transition from environmental to socio-economical

1 optimum PET packaging system. This suggests a trade-off between GWP, revenues, and circularity
2 of the PET packaging system. Additionally, decreased circularity of the system led to increased
3 reliance on V-PET resin to balance for the increased disposal of PET material to landfills in the
4 system as well as to meet the demand for semi-manufacturing products.

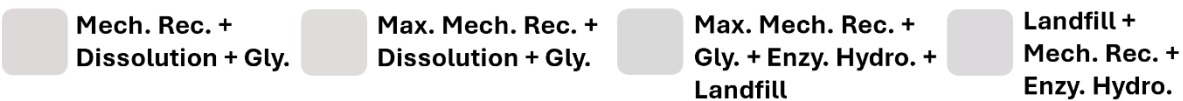
5 The EOL management decisions and selection of recycling technologies along the Pareto frontier
6 curve in Figure 4 are mainly driven by the GWP, revenues, and yield loss factors of recycling
7 technologies, landfilling, and V-PET resin production processes. Minimizing GWP while
8 simultaneously increasing revenues led to selection of recycling technologies having relatively
9 lower GWP, higher revenues, and higher yield loss factors. The recycling technologies with higher
10 yield loss factors lead to increased amounts of V-PET resin into the system due to the associated
11 higher revenues of V-PET resin (see Table 3). Over a certain range of revenues (Figure 4E), the
12 model prescribed higher landfilling rates (up to 42%) of PET packaging material with
13 minimization of GWP and maximization of revenues. This was mainly due to two reasons: 1) lower
14 GWP of landfill operations, and 2) higher revenues from V-PET resin.

15 As mentioned above (Section 3.1), higher landfilling rates demand more V-PET resin into the
16 system to balance for the increased disposal of waste PET at the EOL as well as to meet the demand
17 for semi-manufacturing products. Note that the Pareto-front analysis restricted landfilling up to
18 42% (Figure 4E) mainly due to the epsilon constraints on minimum level of employment and
19 wages as well as the maximum value of CED (see Section 2.4). Also, landfilling rates $\geq 42\%$ and
20 $< 100\%$ would lead to a lower generation of both employment and wages than the observed optimal
21 ranges of constrained epsilon values, which would lead to sub-optimal solutions. To further
22 understand the system behavior and explore this sub-optimal region, an additional Pareto-front
23 analysis was conducted without additional constraints on other objective functions. The results of
24 such analysis are shown in Figure S5 of the SI document (Section S5.1).

25



Legend



1

2 **Figure 4.** Pareto front trade-off plots between GWP and revenues of the U.S. PET packaging
 3 system. Notes: The red and black stars represent environmentally and socio-economically
 4 optimum solutions, respectively, as shown in the pay-off table in Table S1. The data behind this
 5 figure and analysis is shown in Table S2 of the SI document (Section S5).

6 The optimization model predicted the 100% collection and recycling of the total EOL PET
 7 packaging material from \$24.2 up to \$25.1 billion of total system revenues (see Figure 4E) but
 8 differed in the optimal selection of recycling technologies (see Figure 4F). For example, at a
 9 system revenue of \$24.8 billion, the optimum PET packaging system is a combination of

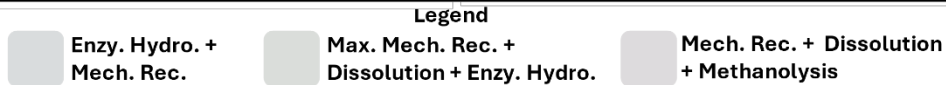
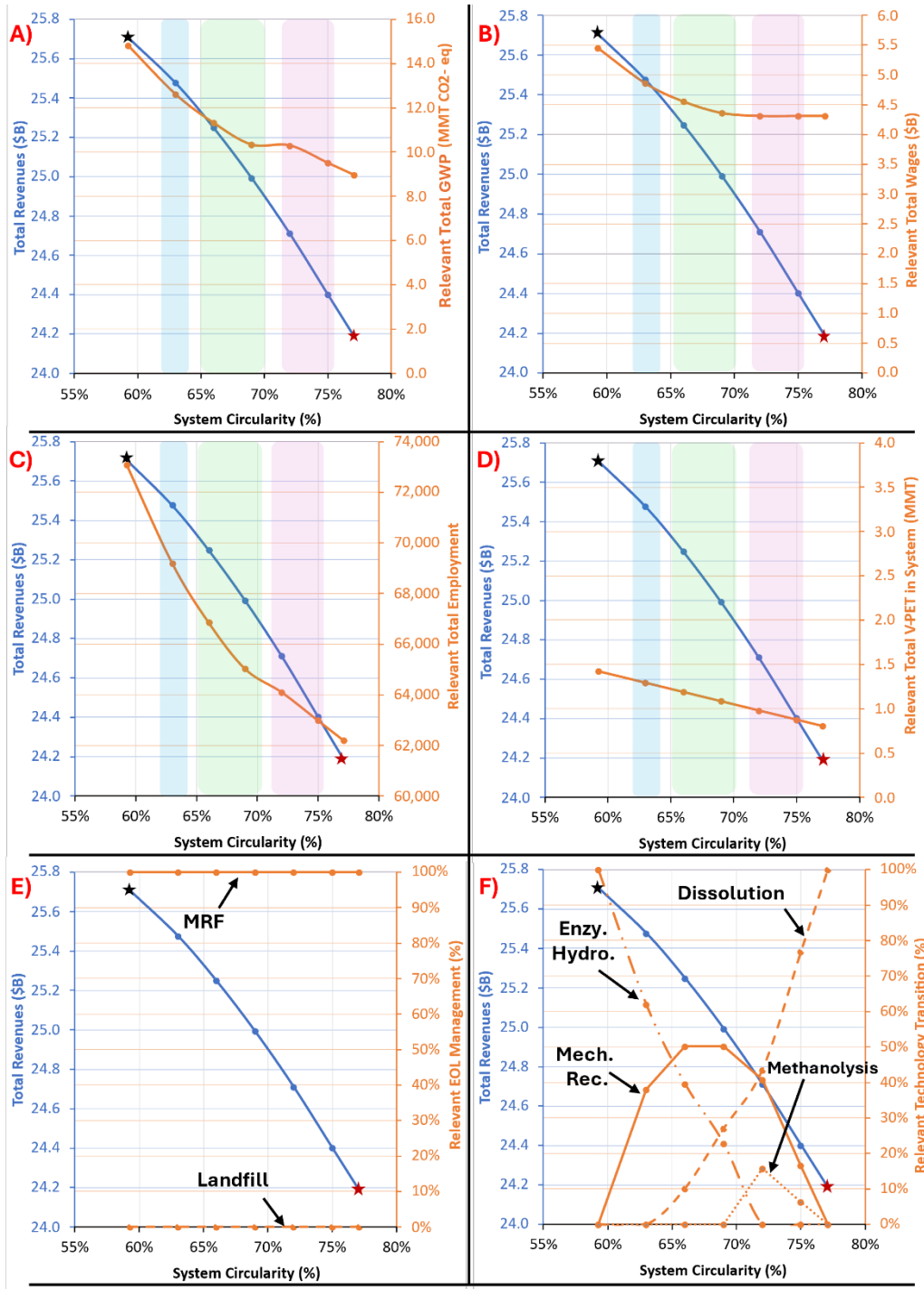
1 mechanical recycling (up to 48%), solvent-based dissolution-precipitation (34%), and glycolysis
2 (18%) recycling technologies (see Figure 4F). This solution led to optimal GWP of 9.28 MMT
3 CO₂-eq. Compared to the environmentally optimum PET packaging system (red star), this is an
4 increase of 3.5% in GWP for a 2.5% increase in the revenue generation. Also, going from \$24.2
5 up to \$25.1 billion of total system revenues led to a gradual increase in the total process waste
6 generation in the system, thereby reducing the system's circularity (to 71%) and increasing the use
7 of V-PET resin (1.011 MMT) to balance for the increased process waste generation or losses of
8 PET material to landfill and WtE processes. Moreover, the employment increased linearly to
9 64,421 employees (by 4%), when compared to the environmentally optimum PET packaging
10 system, however, the wages remained constant until mechanical recycling was maximized to the
11 blend limit of 35%.

12 The total GWP of the PET packaging system increased more sharply beyond \$25.1 billion of total
13 system revenues. This occurred because the optimization model started to predict landfilling of
14 PET packaging material along with a combination of mechanical recycling, and enzymatic
15 hydrolysis (shown by light grey and violet boxes). Increased landfilling leads to the use of
16 economically beneficial V-PET resin into the system to make-up for the material loss and meet the
17 demand for the semi-manufacturing processes. However, this comes at a cost of reduced systems
18 circularity and reduced societal benefits along with increased environmental impacts. The
19 maximum amount of total V-PET was found to be 2.308 MMT (Figure 4D). The decision maker
20 needs to be aware of the trade-offs of decreased societal and environmental benefits along with
21 reduced circularity of the system in the light grey and violet regions. Additional results of the
22 Pareto front analysis are shown in Figures S6-S7 of section S5 of the SI document: GWP-
23 employment (section S5.2) and GWP-wages (section S5.3).

24 **3.4.2 Pareto frontier between revenue and circularity**

25 While the section above explored the trade-offs between GWP and revenues, this section explores
26 the trade-offs between revenues and circularity of the PET packaging system. The results shown
27 in Figure 5 represent an analysis of the system that is optimized on maximizing system's revenue
28 subject to constraints on mass balance, blend limit, circularity, GWP, employment, wages, and
29 energy of the system. Note here that an additional constraint was added on circularity of the system
30 to further understand the system behavior and explore the trade-offs as identified and mentioned
31 in section 3.4.1.

32 The epsilon value of the system's circularity constraint was systematically varied between the
33 identified range shown in Table S1. For a given epsilon value of circularity, the model was solved
34 again to maximize the revenues of the system without violating any of the constraints mentioned
35 above, and the respective values of other system metrics were plotted on the secondary Y-axis as
36 shown in Figure 5 A-C. Similar to Figure 4, the other key results generated from the analysis such
37 as V-PET resin requirements and EOL management decisions are also plotted on secondary Y-axis
38 as shown in Figure 5 D-F. The RHS values of ϵ_{GWP} , $\epsilon_{\text{Employment}}$, ϵ_{Wage} , and ϵ_{CED} for the GWP,
39 employment, wages, and CED constraints were 14.81 MMT CO₂-eq, 62200 employees, \$4.31
40 billion, and 301.49 PJ, respectively.



1
2
3
4

Figure 5. Pareto front trade-off plots between revenues and circularity of the U.S. PET packaging system. Notes: The red and black stars represent environmentally and socio-economically optimum solutions, respectively, as shown in the pay-off table in Table S1. The

1 simplified approach and data behind this figure and analysis is shown in Table S3 of the SI
2 document (Section S5.4).

3 Overall, a trend similar to that identified in Figure 4 was also observed in Figure 5 wherein
4 increased circularity led to decreased socio-economic and environmental impacts of the PET
5 packaging system. Also, increased circularity led to a linear decrease in the requirement of V-PET
6 resin into the system. However, the key difference between Figure 4 and 5 is in terms of the EOL
7 management decisions for PET packaging material (Figure 4E and 5E) and the Pareto optimal
8 selection of the recycling technologies (Figure 4F and 5F). Maximizing revenues while
9 simultaneously increasing circularity always led to 100% collection and recycling of the PET
10 packaging material with zero percent landfilling at the EOL (see Figure 5E). This finding from the
11 perspective of revenues and circularity further states that collection and recycling via a suite of
12 recycling technologies generates more revenues and results in higher circularity than landfilling or
13 WtE processes only.

14 The model selected enzymatic hydrolysis, mechanical recycling, dissolution-precipitation, and
15 methanolysis processes as recycling technologies for the Pareto-front analysis between revenues
16 and circularity (Figure 5F). The selection of these recycling technologies is mainly driven by their
17 revenue and yield loss factors. The yield loss factor is a key parameter in determining the
18 circularity of the system, wherein the lower the yield loss factor for recycling technologies the
19 higher the circularity of the PET packaging system. It is important to note that methanolysis and
20 glycolysis have similar revenues and yield loss factors (see Table 3), therefore, there is no “tie-
21 breaker” for the same and the model can select either of these two technologies resulting in similar
22 revenues and circularity of the system. However, the decision maker needs to be aware that
23 selection of methanolysis leads to higher environmental impacts than glycolysis process.
24 Therefore, the combination of mechanical recycling, dissolution-precipitation, and methanolysis
25 recycling technologies at the circularity of 72% and 75% (see Table S3) is a sub-optimal Pareto-
26 front solution relative to the analysis shown in Figure 4. Additional results of the Pareto-front
27 analysis between revenues-circularity and wages-circularity without additional constraints on
28 other system metrics are shown in Figures S8-S9 of the SI document (Section S5.5-S5.6),
29 respectively.

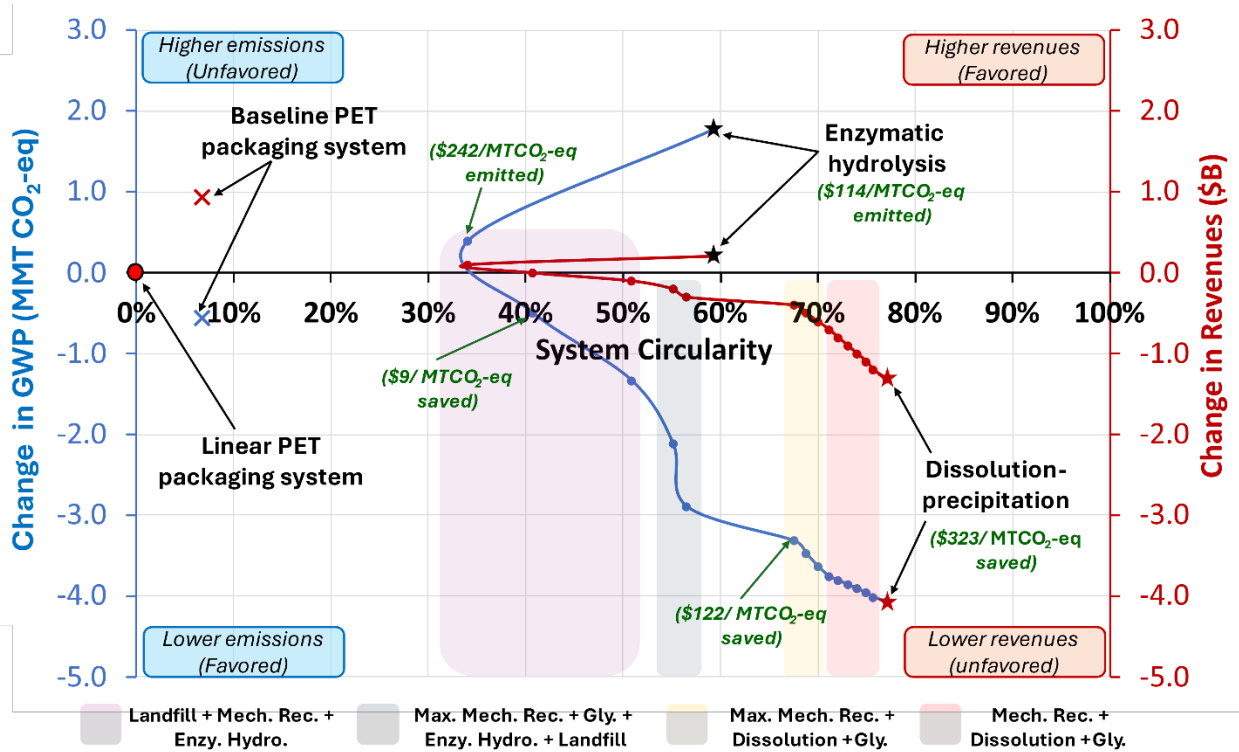
30 Overall, using the ϵ -constraint method to conduct rigorous Pareto-front analysis provided deeper
31 insights into material flows through system processes and the resulting relationships among the
32 studied system metrics. However, this method has a number of limitations, based on (Branke 2008,
33 Mavrotas 2009, Gunantara 2018), which are briefly summarized here: 1) computationally (time)
34 intensive process, as it requires solving the optimization model for each varied epsilon value,
35 especially in our case with five different objective functions; 2) manual selection of equidistant
36 grid points for the epsilon values can lead to limited number of Pareto-optimal solutions; 3) unable
37 to determine a solution outside of a feasible design space (or constraints); 4) visualizing Pareto-
38 optimal solutions become challenging with increased objective functions, especially in our case
39 with five different objective functions. Despite these limitations, the information obtained using ϵ -
40 constraint method is useful to identify/generate alternative Pareto-optimal system designs for
41 decision makers. Overall, these Pareto-optimal system designs provide the decision makers with

1 quantitative information and understanding of the system material flows and relevant impacts in
 2 the context of system analysis.

3 3.5. Pareto Optimal Decision Diagram: GWP, Circularity, and Revenues

4 A new decision diagram was developed to guide and help decision makers to visualize the trade-
 5 offs between important system metrics of alternative PET packaging systems relative to linear
 6 economy, as shown in Figure 6. This analysis leverages the Pareto-front analysis results shown in
 7 Figure 4. Moreover, this figure could aid decision makers to identify favorable and unfavorable
 8 alternative PET packaging system designs with the transition from linear to circular PET
 9 packaging.

10 Figure 6 shows the change in GWP (primary Y-axis) and revenues (secondary Y-axis) relative to
 11 the linear economy scenario as a function of PET packaging system's circularity. The current US
 12 baseline PET packaging system based on our prior work (Chaudhari, Watkins et al. 2025) is also
 13 shown, which exhibits slightly favorable revenue and lower GWP compared to the linear economy
 14 configuration.



15

16 **Figure 6.** Change in GWP and revenues compared to the linear PET packaging system as a
 17 function of system's circularity. Note: The red and black stars represent environmentally and
 18 socio-economically optimum solutions, respectively, as shown in the pay-off table in Table S1.

19 The Pareto-optimal system configuration above the X-axis represents higher emissions
 20 (unfavorable) and higher revenues (favorable) than the linear economy, whereas the system
 21 configuration below represents lower emissions (favorable) and lower revenues (unfavorable),
 22 compared to the linear economy. The Pareto-optimal and socio-economically optimal system

1 configuration above X-axis may not be the best solution in an era where industries are working
2 towards mitigating global warming.

3 On the other hand, the system configurations below X-axis shows savings of GWP along with
4 enhanced circularity with a relatively modest loss in revenues until 68% of circularity. At higher
5 system circularity (> 68%) there is a sharp decrease in the systems revenues for a relatively small
6 savings of GWP. From the metrics presented in Figure 6, a reasonable policy objective would be
7 to target PET packaging system circularity up to 68%. It is further justified to encourage
8 investment in recycling programs to collect PET for recycle, to build out mechanical recycling up
9 to the blend limit, and achieve greater circularity by supporting emerging advanced recycling such
10 as dissolution-precipitation as well as glycolysis.

11 A decision maker could further benefit from understanding the cost of GWP savings of various
12 PET packaging system designs, as a function of systems circularity. For example, system
13 technology configurations with circularity of 41% to 68% represents a loss in U.S. revenues
14 ranging from \$9/MT CO₂-eq saved to \$122/MT CO₂-eq saved. These costs represents “willingness-
15 to-pay” (WTP) for reducing global warming and addressing climate change. These costs are
16 modest compared to (Kotchen, Turk and Leiserowitz 2017) that provide an average U.S. WTP
17 estimate of \$177 per year in support of addressing climate change.

18 **3.6 Scenario Analysis of PET Packaging Systems in Circular Economy**

19 Scenario analysis was conducted using the same system optimization model (as described in
20 Section 2.2) to understand the impacts of various system configurations (see Table S4) as well as
21 to validate the optimization results. Additional results of the scenario analysis are presented in
22 Section S6 of the SI document. The MFA results in the form of sankey diagrams are is shown in
23 Figure S10 and summary of key system metrics shown in Figure S11 (section S6.1). Moreover,
24 carbon and energy intensity of each scenaio was also evaluated and shown in Figure S12 (section
25 S6.2).

26 **3.7 Future Research Directions**

27 The present study utilized the ϵ -constraint method to conduct rigorous Pareto-front analysis
28 between conflicting environmental and socio-economic impacts for the U.S. PET packaging
29 systems. Even though this method is useful to generate alternative Pareto-optimal solutions for
30 decision makers, future research work could investigate applications of multi-criteria decision-
31 making methods to aid the selection process among the identified Pareto-optimal PET packaging
32 system designs.

33 While the present study focused on U.S. PET packaging material in a closed-loop circular
34 economy, future system modeling should include PET fiber/textile applications with careful design
35 of the system material flows, as noted out earlier by (Chaudhari, Watkins et al. 2025). In addition
36 to recycling as a circular economy strategy, future system modeling could consider additional
37 strategies including, but not limited to, reuse, repair, and refurbish, as well as open-loop PET
38 material flows to different applications. Including different applications of PET material also
39 brings in the supply and demand perspectives with considerations of price elasticities and

1 availability of recyclate, further demanding a complex system model with potentially adding multi-
2 material dimensions. Integrating consumer behavior in the system optimization model could
3 further highlight and quantify the role of consumers in achieving a sustainable and optimal
4 circular economy.

5 In addition to plastics, the system analysis framework presented here could be applied to other
6 materials supply chain processes including, but not limited to, metals, papers, textile, rubbers, and
7 glass, to evaluate the sustainability implications of implementing circular economy via emerging
8 manufacturing technologies. This would require sufficient availability of the required information
9 and input data aligning with the research scope and objectives.

10 **4. CONCLUSION**

11 Using systems analysis and optimization techniques, the present study rigorously quantified
12 Pareto-frontier trade-offs between conflicting environmental and socio-economic impacts as well
13 as trade-offs between the socio-economic impacts and systems circularity of the U.S. PET
14 packaging material flows in a circular economy. Furthermore, our study revealed the transition of
15 recycling technologies along with changes in EOL management decisions, optimal need of V-PET
16 resins in the system, and circularity of the systems via the Pareto front trade-off analysis of circular
17 PET packaging systems.

18 Both environmentally and socio-economically optimal circular PET packaging systems predicted
19 by the optimization model outperformed the linear economy, except in terms of a small reduction
20 in U.S. revenues for the environmentally optimal system. Minimizing environmental impacts of
21 the U.S. PET packaging system showed 31% savings of GWP, 37% savings of energy, 29% higher
22 employment, 32% higher wages, but resulted in 5% lower revenues, when compared with a linear
23 economy. However, the environmentally optimal system showed 15% lower employment, 21%
24 lower wages, and 6% lower revenues but had the highest circularity of 77% with 39% lower GWP
25 and 37% lower CED, when compared with socio-economically optimal system.

26 This study demonstrates that the environmental and socio-economic sustainability of the U.S. PET
27 packaging systems depends on the performance of the processes involved within the system.
28 Moreover, a more sustainable circular economy for U.S. PET packaging is attainable with higher
29 process efficiency (or minimizing loss of PET material during processing), higher quality of
30 recycled resins from recycling technologies, and lower environmental impacts of emerging
31 recycling technologies compared to traditional fossil-based production of V-PET resins. The
32 results showed that V-PET resin would still be required in circular PET packaging systems due to
33 loss of PET material to landfilling and incineration during the processing steps.

34 The EOL management decisions prescribed by the optimization model and selection of recycling
35 technologies along the Pareto-frontier curves are mainly driven by the relevant environmental,
36 socio-economic, and process yield loss factors. The sensitivity analysis and Pareto-front analysis
37 revealed that multiple recycling technologies, including mechanical and advanced/chemical
38 recycling, would be required to balance the trade-offs between circularity, environmental, and
39 socio-economic impacts of the systems. However, there is not a unique set of recycling
40 technologies to achieve a “win-win” sustainable circular economy of PET packaging systems in

1 the U.S., instead it depends on the decision makers objectives and targeted metrics of the system.
2 Finally, the Pareto optimal decision diagram helped to visualize the relationship between GWP,
3 revenues, and circularity of various Pareto optimal system designs relative to linear economy along
4 with the loss in revenues due to savings of GWP.

5 These results are based on early-stage impact data for emerging advanced/chemical recycling
6 technologies for U.S. PET packaging and estimated socioeconomic impact factors in this emerging
7 industry. Systems analysis and optimization can be improved in the future with updated data from
8 research and development leading to industrial commercialization of these emerging technologies.
9 Overall, systems analysis framework used in this study demonstrated the effects of systems
10 parameters on sustainability performance metrics of the system as well as helped to better
11 understand the inter-relationships among the system processes. Systems analysis approach
12 provides insights into improvement for sustainability of future circular economy technologies
13 compared to traditional technologies.

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26 **CRedit Authorship Contribution Statement**

27 **Utkarsh S. Chaudhari:** Writing – original draft, Writing – review & editing, methodology,
28 conceptualization, investigation, formal analysis, validation, visualization. **David W. Watkins:**
29 Writing – review & editing, methodology, validation, supervision. **Robert M. Handler:** Writing
30 – review & editing, supervision. **Barbara K. Reck:** Writing – review & editing, supervision. **Anne**
31 **T. Johnson:** Writing – review & editing, supervision. **Tasmin Hossain:** Writing – review &
32 editing, supervision. **Damon S. Hartley:** Writing – review & editing, supervision. **Vicki S.**
33 **Thompson:** Writing – review & editing, supervision. **David R. Shonnard:** Writing – review &
34 editing, conceptualization, methodology, project administration, funding acquisition, supervision,
35 validation, resources.

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