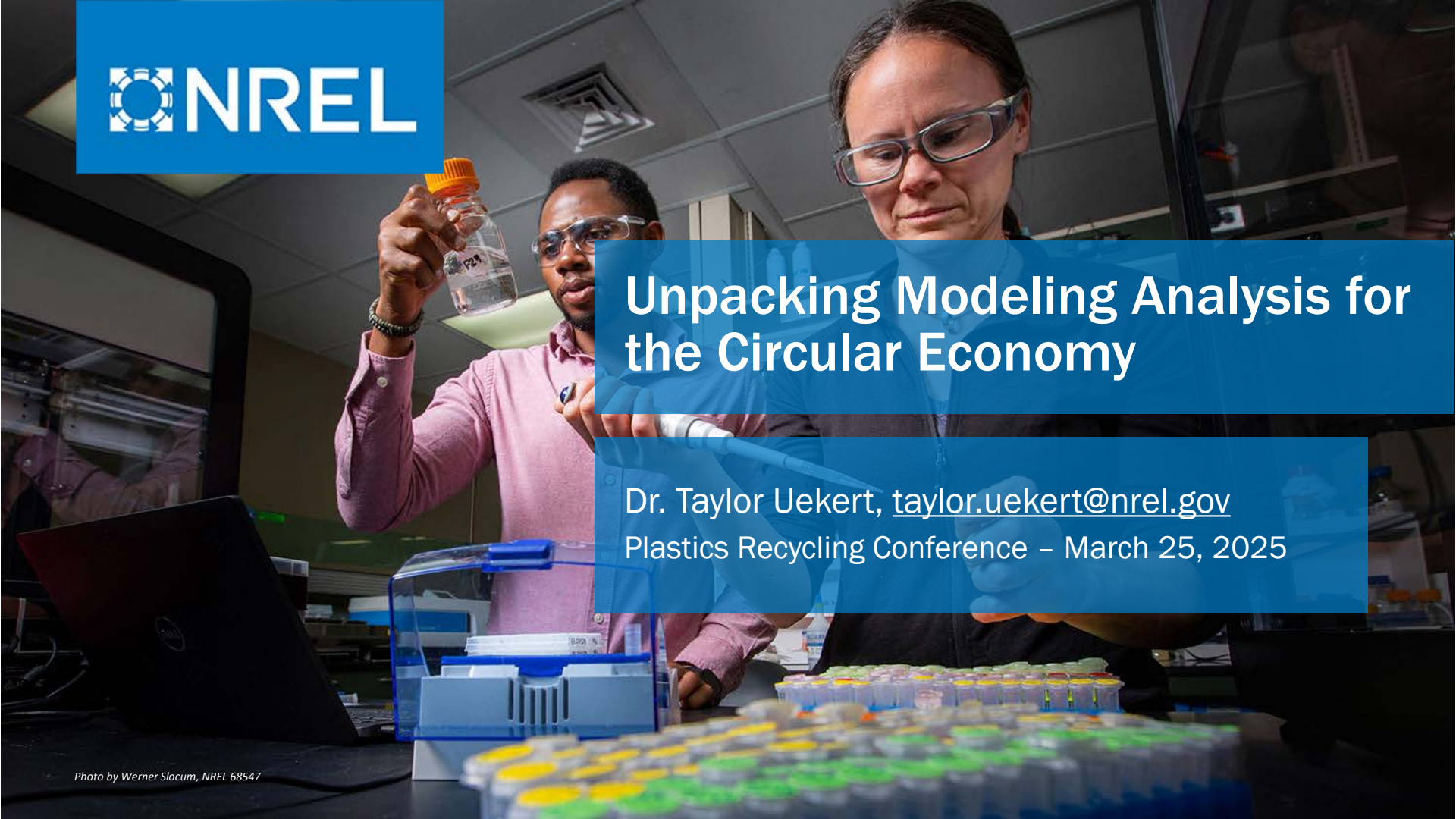


Unpacking Modeling Analysis for the Circular Economy

Dr. Taylor Uekert, taylor.uekert@nrel.gov

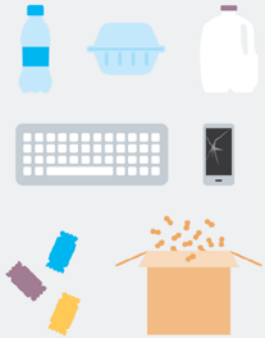
Plastics Recycling Conference – March 25, 2025

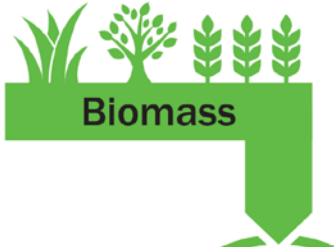
Photo by Werner Slocum, NREL 68547

Analysis-Guided R&D, **Characterization**, and **Modeling**

Mission: Develop robust processes to recycle existing waste plastics and create new circular polymers.

Plastics Waste





Deconstruction

Building Blocks

Redesign

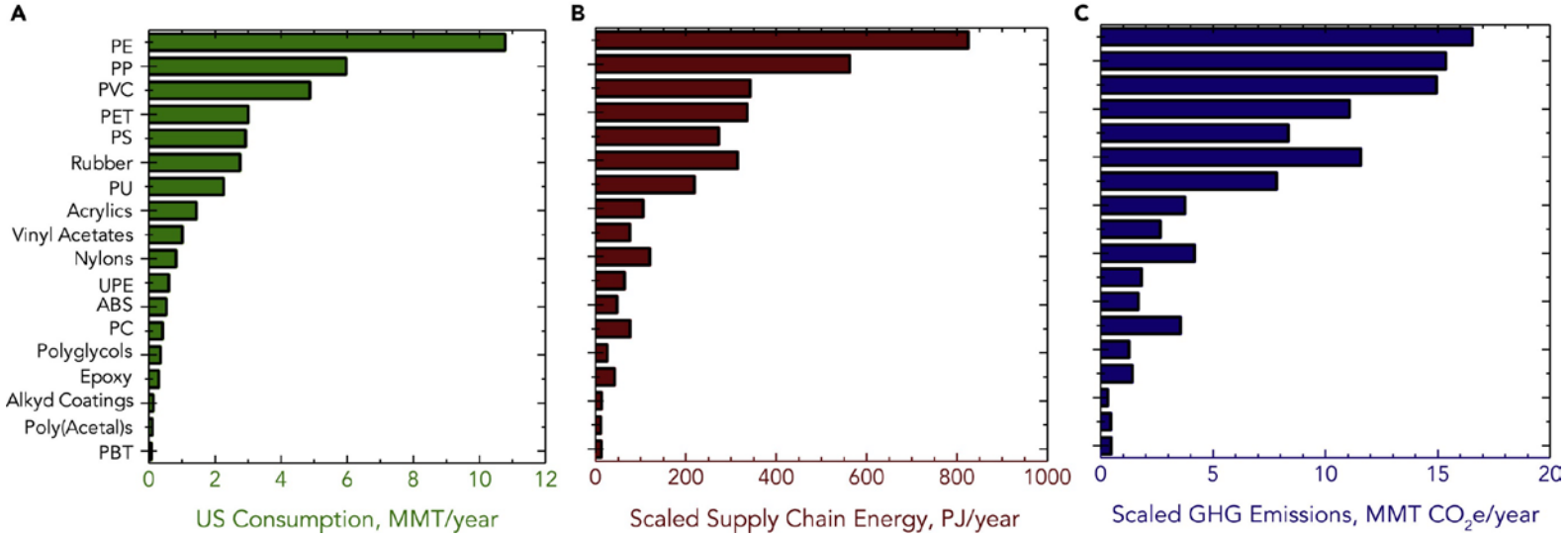
Circular Polymers

Plastics waste and biomass converted to building blocks

Conversion of building blocks into circular and biodegradable polymers

Why plastics?

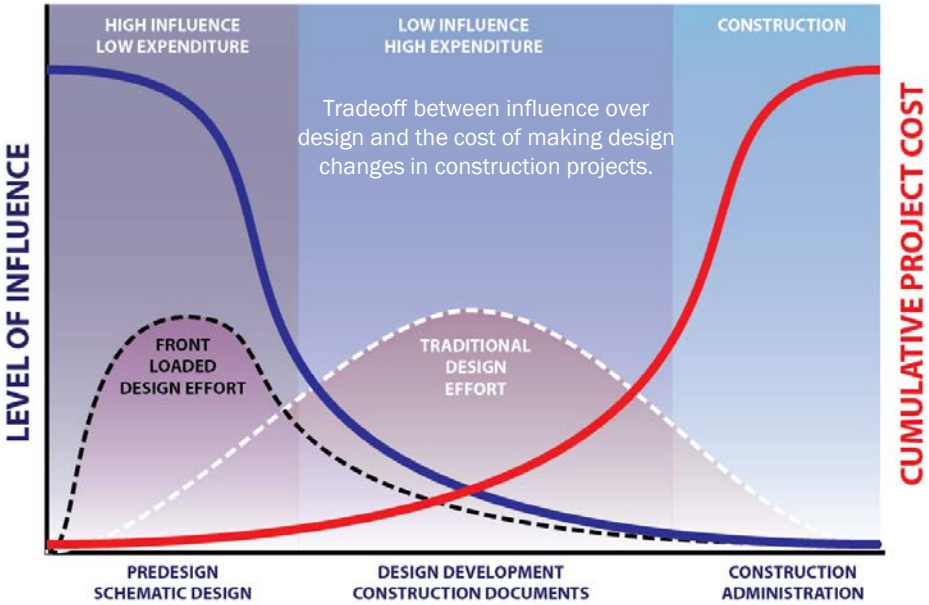
- Plastic production and disposal in the U.S. today have known implications: 2% of total U.S. greenhouse gas (GHG) emissions and 44 million metric tons (MMT) of landfilled or incinerated waste.
- Recycling could reduce waste *and* the impacts associated with virgin plastic production.



S. R. Nicholson, et al., *Joule*, 2021, *5*, 673-686; A. Milbrandt et al., *Resourc. Conserv. Recycl.*, 2022, *183*, 106363. Abbreviations: PE – polyethylene; PP – polypropylene; PVC – polyvinyl chloride; PET – polyethylene terephthalate; PS – polystyrene; PU – polyurethane.

Why analysis-guided research?

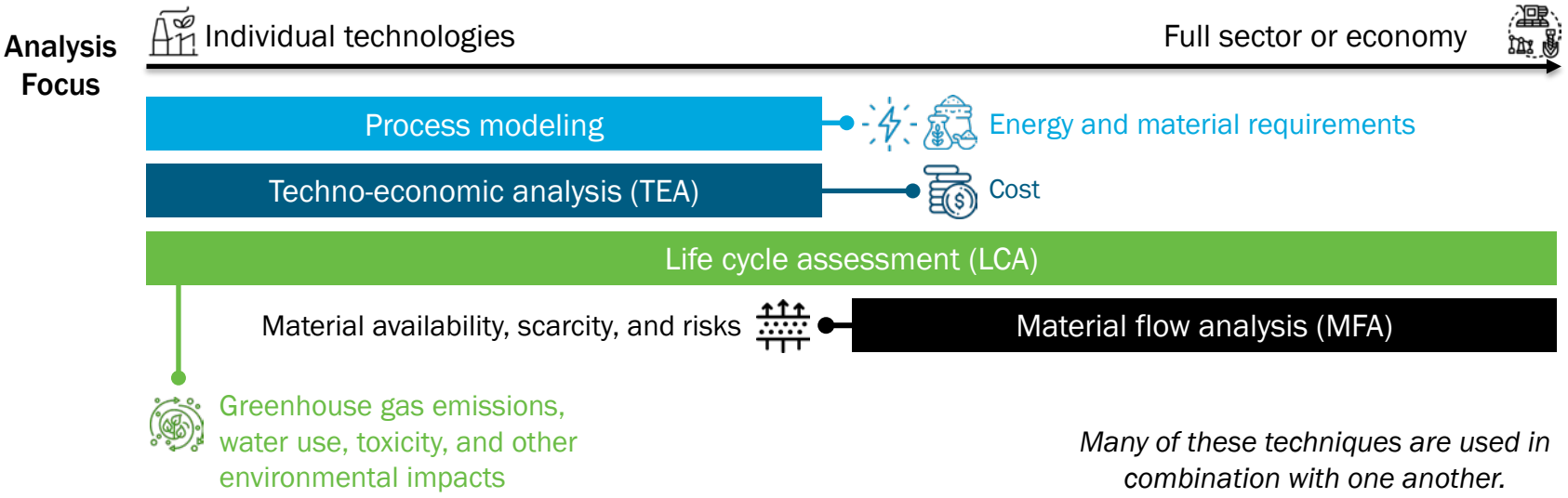
- As we design a circular future, innovations should mitigate harms rather than causing more.
- Negative impacts can be “locked in” by early-stage R&D decisions. More opportunities exist to address impacts the earlier they are considered.



Wheeler Kearns Architects; Paulson, 1976

Analysis methods

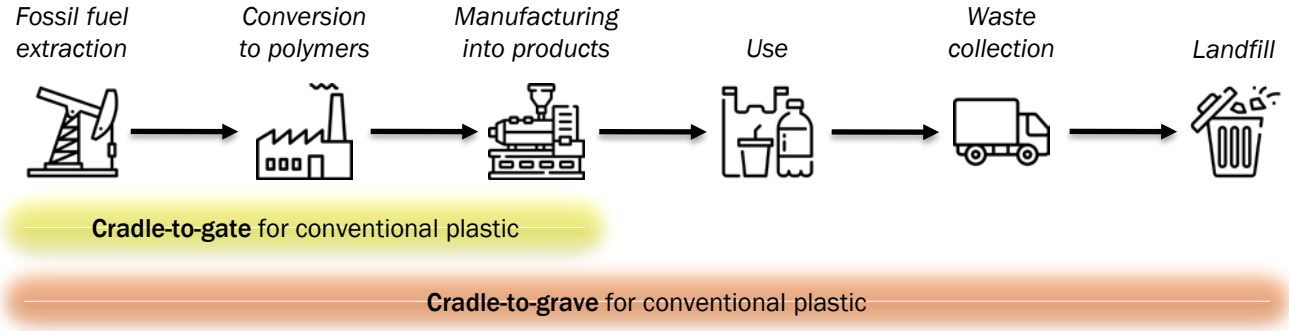
Types of analysis



Many of these techniques are used in combination with one another.

Define goal and scope

- What are you evaluating (feedstocks, technologies, etc.)?
- What are you comparing to?
- What is your **system boundary** and is it consistent?
- What is your **functional unit** and is it consistent?



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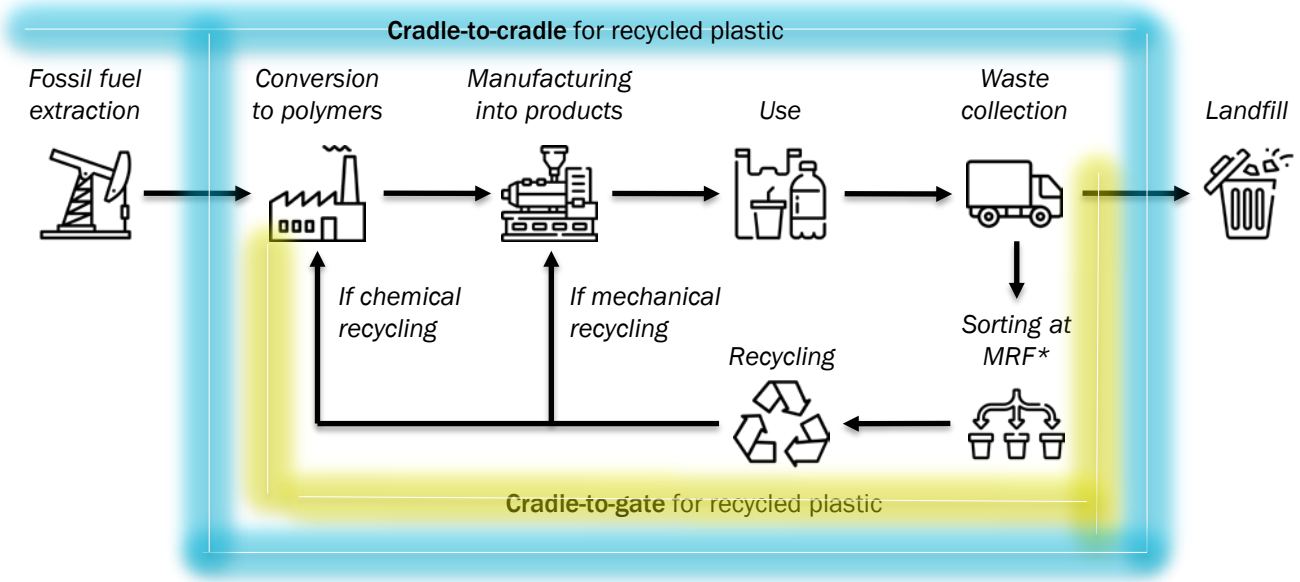
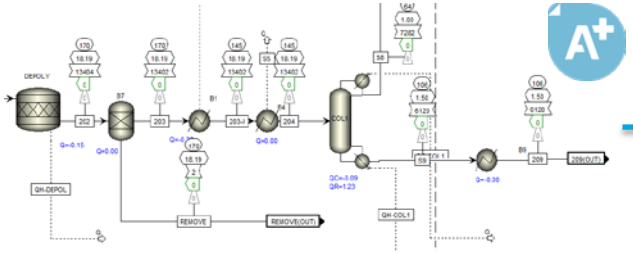


* MRF = materials recovery facility

Analysis methods

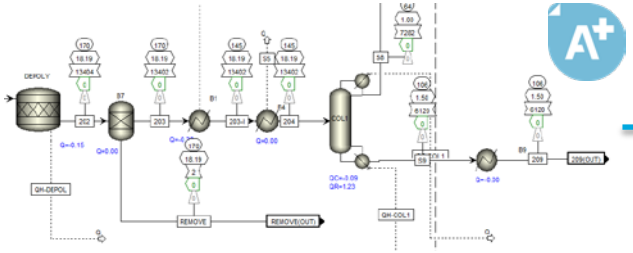
Collect data & build process model



Material and energy flows (aka **life cycle inventory** or **foreground data**)

Analysis methods

Collect data & build process model



Material and energy flows (aka **life cycle inventory** or **foreground data**)

TEA

Discounted cash flow analysis

- Use prices from proprietary databases to calculate **operational expenses** (**OPEX**) and Aspen estimates or company quotes to determine **capital expenses** (**CAPEX**).
- Calculate **minimum selling price** (**MSP**) in $/kg.

DCFROR Worksheet

Year	-2	-1	0	1	2	3
Fixed Capital Investment	$4,132,723	$30,995,420	$16,530,891			
Land	$140,000					
Working Capital			$6,457,379			
Loan Payment				$11,548,079	$11,548,079	$11,548,07
Loan Interest Payment	$495,927	$4,215,377	$6,199,084	$6,199,084	$5,771,164	$5,309,01
Loan Principal	$6,199,084	$52,692,214	$77,488,550	$72,139,555	$66,362,640	$60,123,57
Product Sales				$56,138,569	$74,851,426	$74,851,42
By-Product Credit				$4,558,581	$6,078,108	$6,078,10
Total Annual Sales				$60,697,150	$80,929,533	$80,929,53
Annual Manufacturing Cost						
Feedstock				$12,934,688	$17,246,250	$17,246,25
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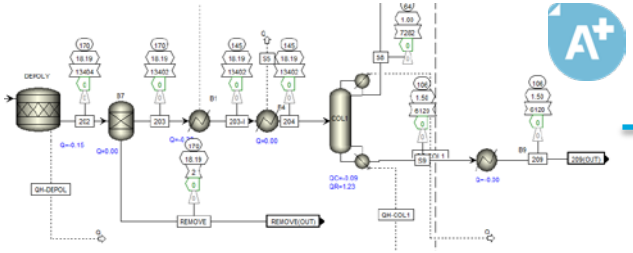
Steam Plant Writedown				3.75%	7.22%	6.68%
Depreciation Charge				$548,731	$1,040,942	$962,78
Remaining Value				$13,870,750	$12,837,808	$11,875,01
Net Revenue				($16,410,748)	($18,549,681)	($8,969,643
Losses Forward				($16,410,748)	($34,960,429)	($34,960,429
Taxable Income				($16,410,748)	($34,960,429)	($43,929,472
Income Tax				$0	$0	$-

Analysis methods

Collect data & build process model



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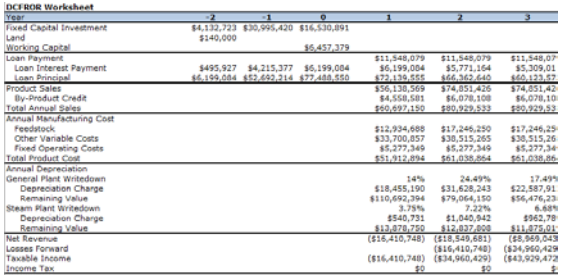

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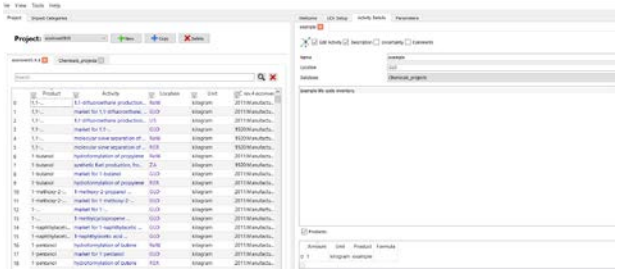
Impact assessment

- Link life cycle inventory to **background data** (e.g., ecoinvent)[1] in an LCA software (e.g., Brightway)[2]
- Use an **assessment methodology** (e.g., ReCiPe)[3] to estimate environmental impacts.



[1] https://ecoinvent.org/; [2] B. Steubing, et al., *Software Impacts*, 2020, *3*, 100012. [3] M. A. J. Huijbregts, et al., *Int. J. LCA*, 2017, *22*, 138-147.

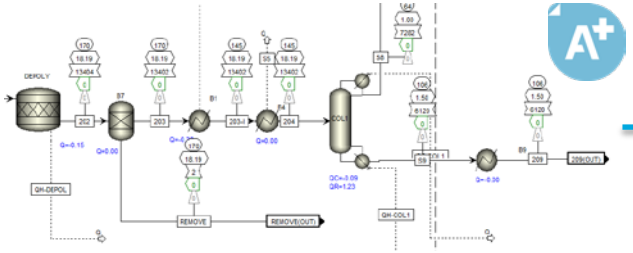
Analysis methods

Additional market data → **Circularity analysis**

- Explore material losses and impacts across entire sector

MFA

Collect data & build process model



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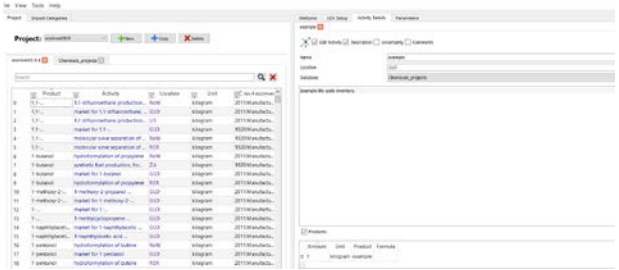

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Filling data gaps

Process modeling

Problem: missing thermodynamic properties

Solutions: literature search, experimental validation, proxy assumptions

TEA

Problem: unknown cost

Solutions: tools (e.g., CatCost),[1] model the new material's production, proxy assumptions

LCA

Problem: unknown environmental impacts

Solutions: model the new material's production, estimate based on precursors, proxy assumptions

MFA

Problem: missing production and/or end-of-life data

Solutions: "backfill" using differences between known data points, proxy assumptions

[1] https://catcost.chemcatbio.org/

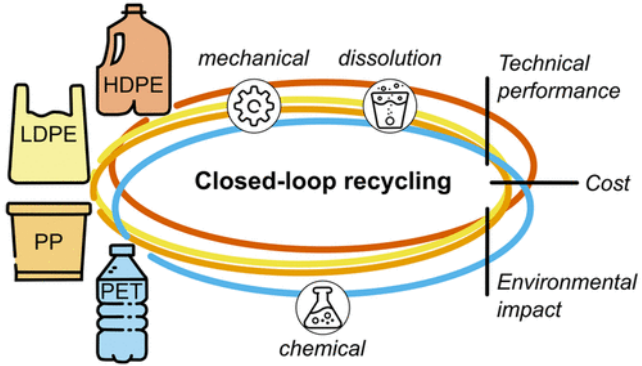
Analysis examples

Comparing recycling options

System boundary: cradle-to-gate
Functional unit: kilogram of virgin or recycled plastic

Research question: How do closed-loop mechanical and chemical recycling strategies for common plastics compare across environmental, economic, and technical parameters?

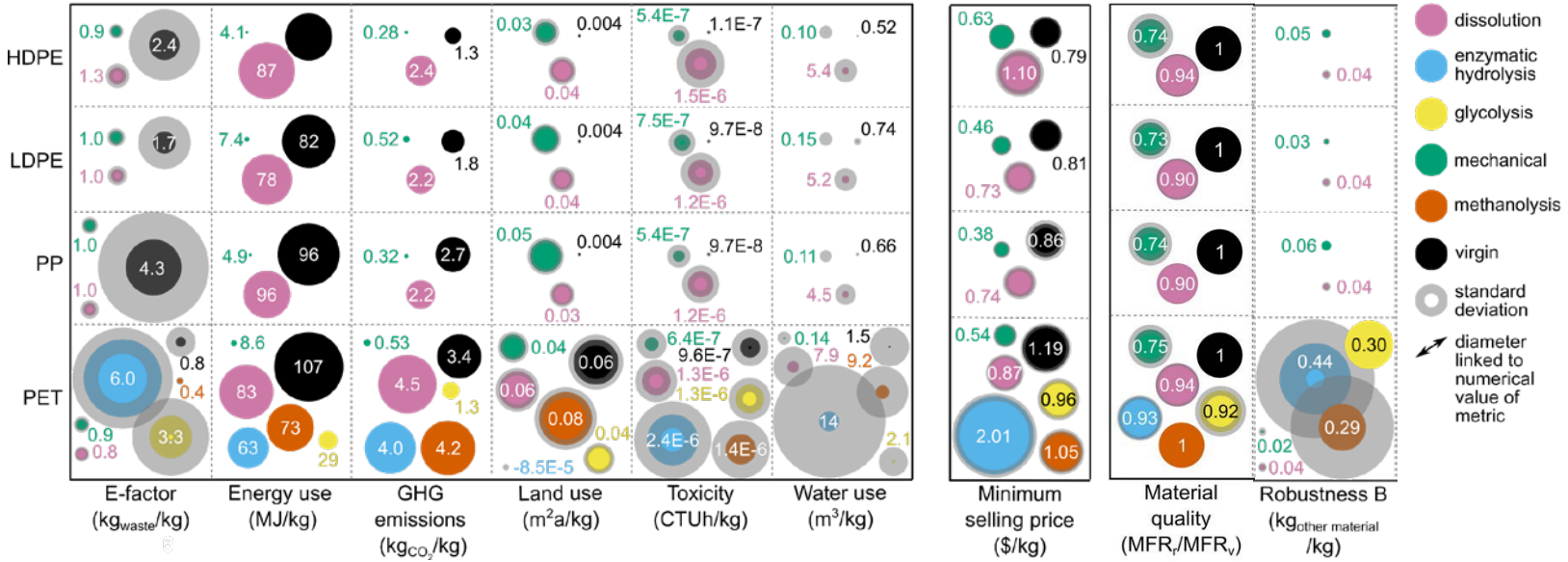
Approach: TEA and LCA on a consistent basis



T. Uekert et al., *ACS Sus. Chem. Eng.*, 2023, *11*, 965.

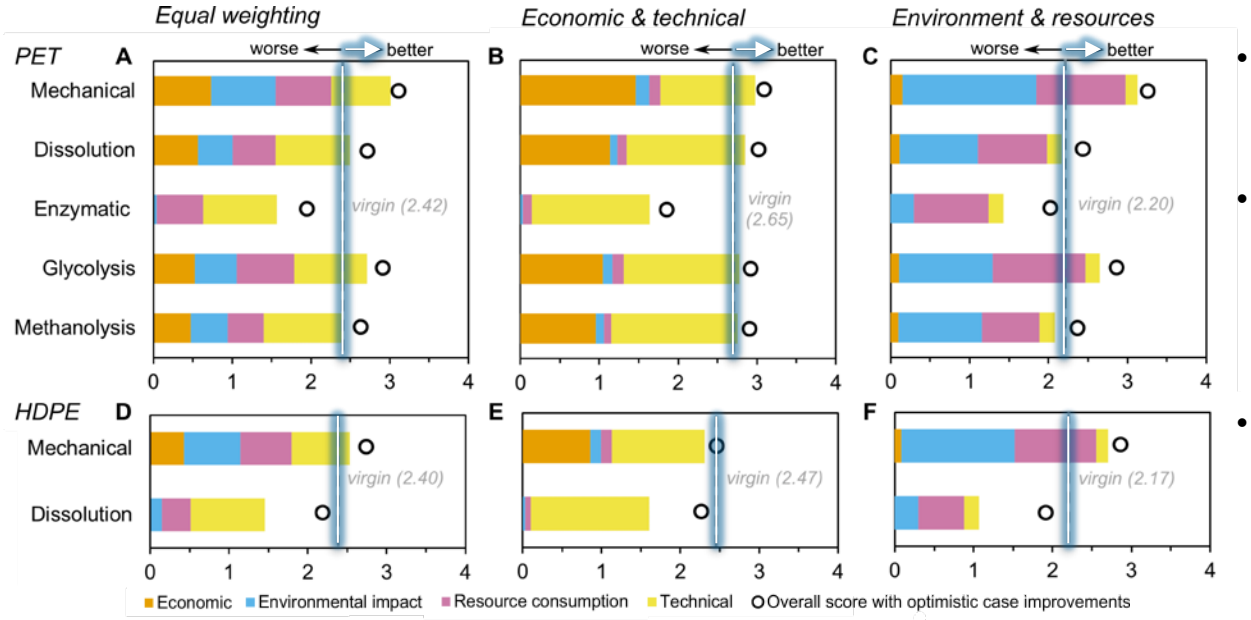
Comparing recycling options

Quantification of tradeoffs between price / environmental impacts and technical constraints across recycling options.



T. Uekert et al., *ACS Sus. Chem. Eng.*, 2023, *11*, 965. Abbreviations: HDPE – high density polyethylene; LDPE – low density polyethylene; PP – polypropylene; PET – polyethylene terephthalate

Comparing recycling strategies

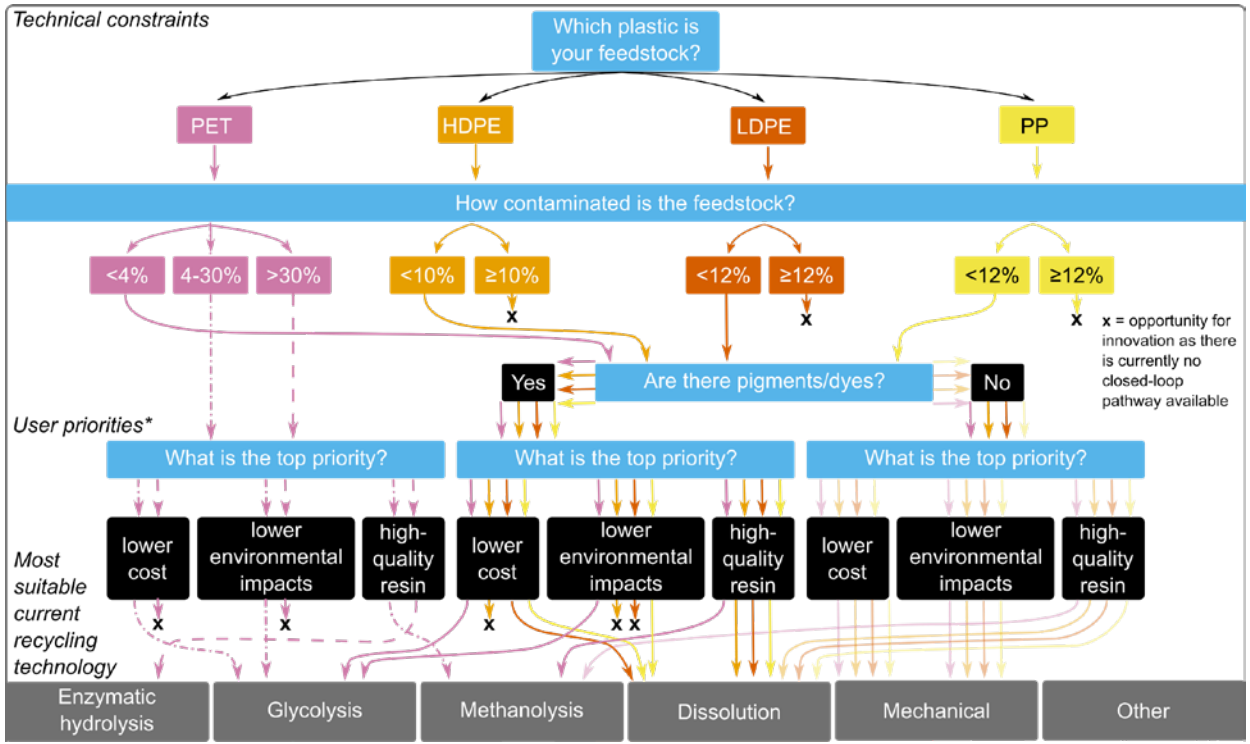


- Multi-criteria decision analysis (MCDA) – allows for evaluation across conflicting criteria.
- Mechanical recycling and glycolysis offer economic, environmental, and technical benefits relative to virgin plastic.
- Process improvements can enable technologies with low scores to improve to similar or better than virgin plastic manufacturing.

T. Uekert et al., *ACS Sus. Chem. Eng.*, 2023, *11,* 965. Abbreviations: PET – polyethylene terephthalate; HDPE – high density polyethylene

Comparing recycling strategies

Analysis results can be synthesized to identify recycling options for different priorities.



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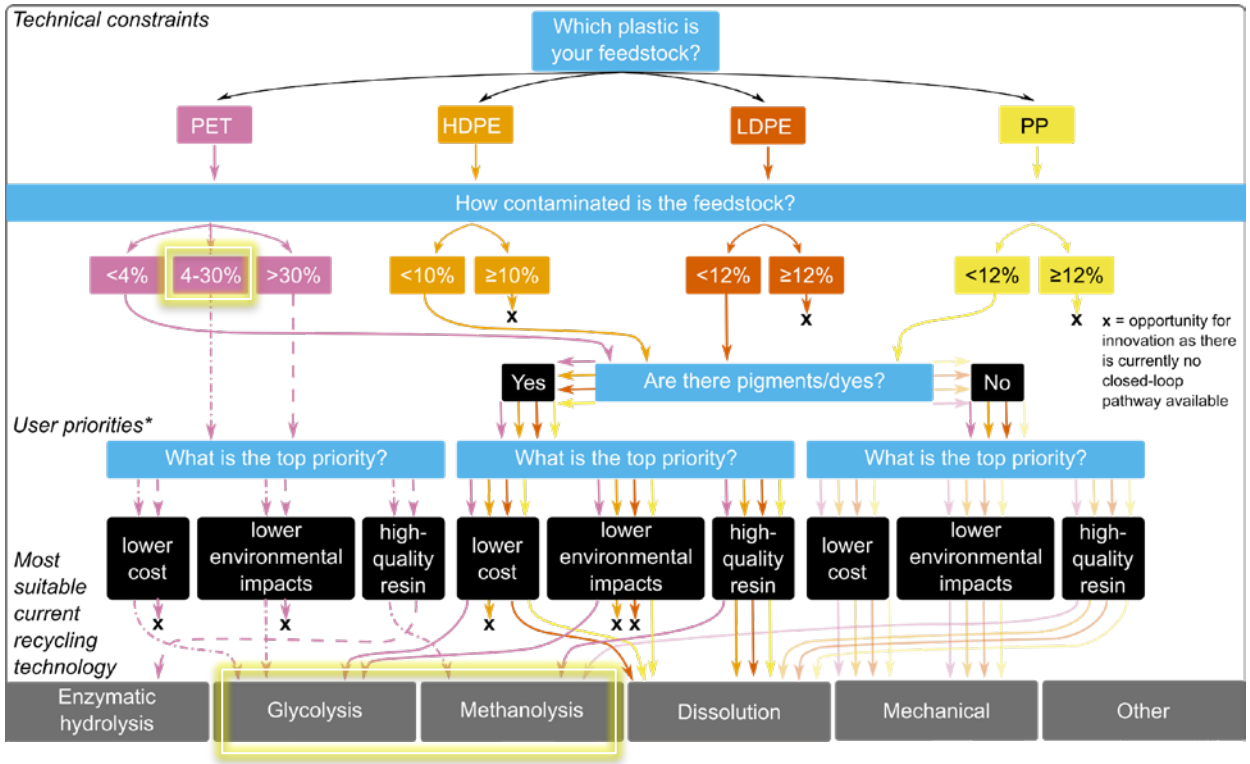

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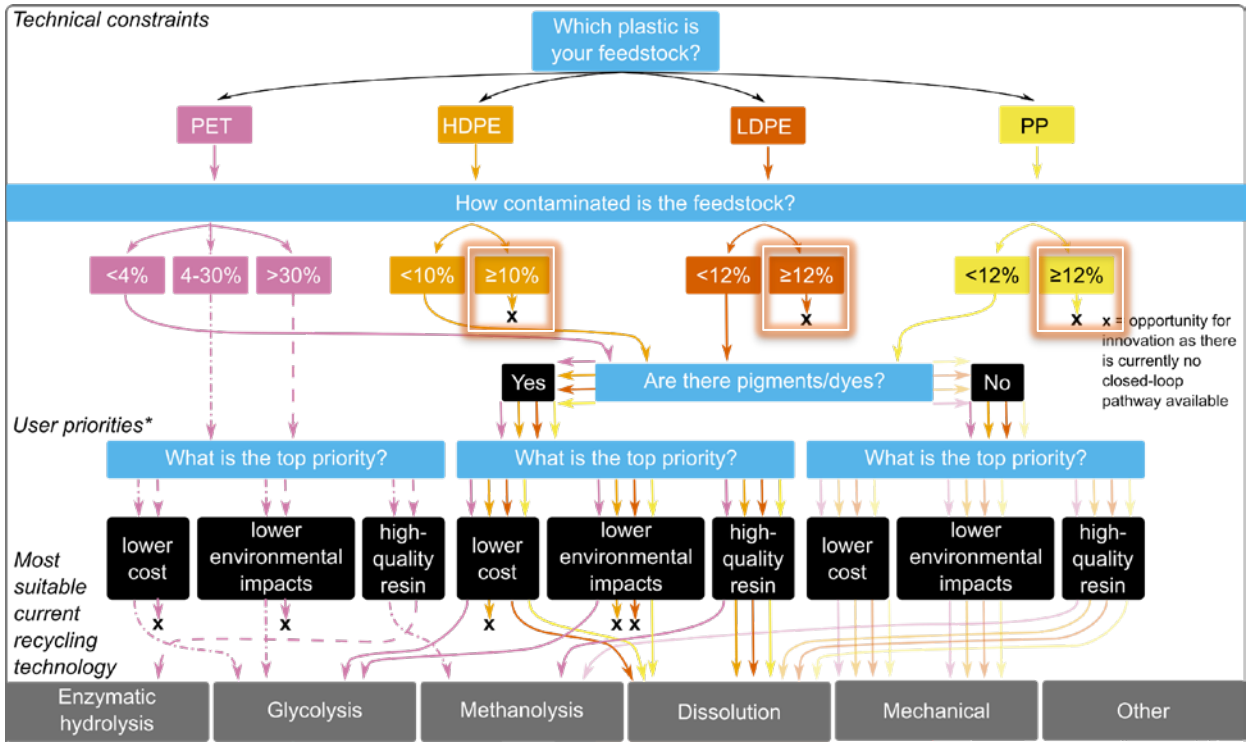


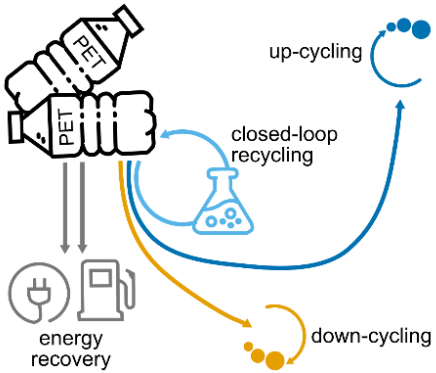
T. Uekert et al., *ACS Sus. Chem. Eng.*, 2023, *11*, 965.

Optimizing across multiple pathways

System boundary: cradle-to-grave / cradle-to-cradle
Functional unit: all PET produced in a year in the U.S.

Research question: What combination of recycling options could reduce costs and environmental impacts while increasing circularity for PET?

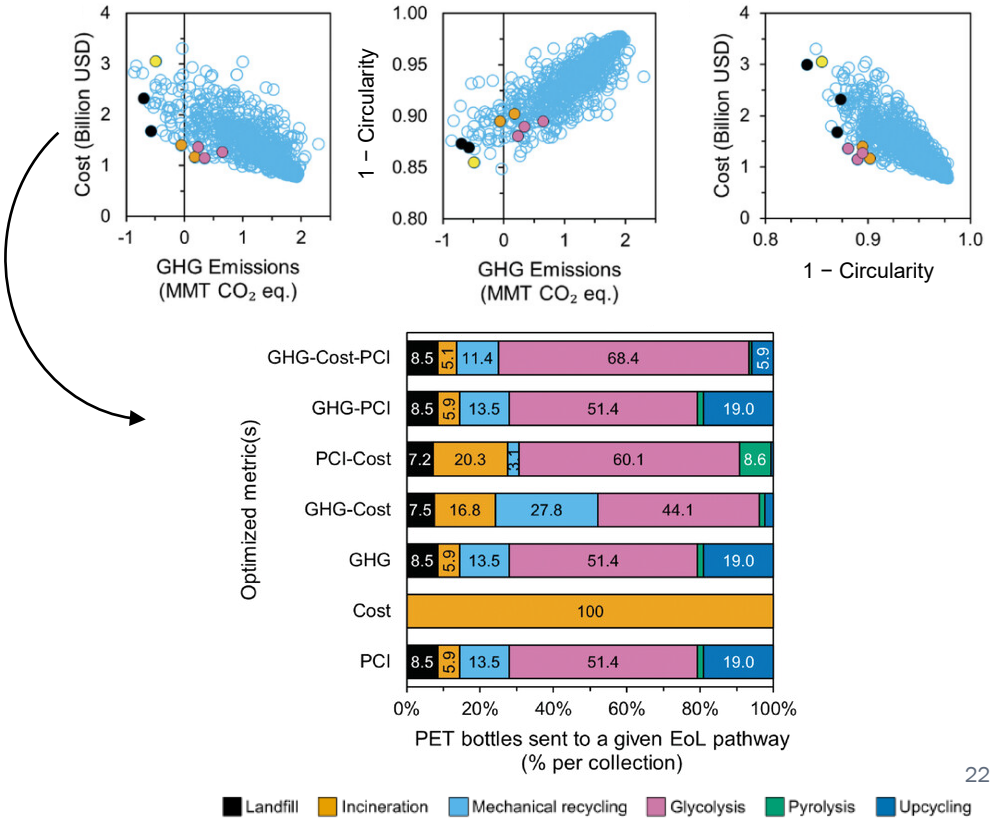
Approach: Python-based material flow model that dynamically tracks PET from production to end-of-life with multiple end-of-life options



T. Ghosh and T. Uekert *et al. Adv. Sustain. Syst.* 2023, *8*, 2300068

Optimizing across multiple pathways

- Monte Carlo analysis allows the model to screen thousands of combinations of end-of-life pathways and determine a local optimum based on criteria.
- Optimal strategies require multiple end-of-life pathways in parallel, especially mechanical recycling and glycolysis.

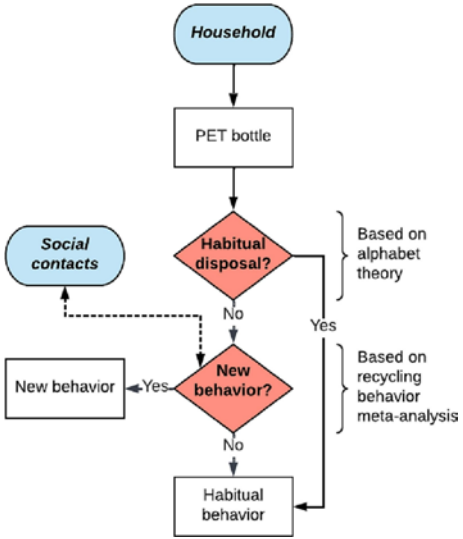


T. Ghosh and T. Uekert *et al. Adv. Sustain. Syst.* 2023, *8*, 2300068. Abbreviations: PCI – plastic circularity index; EoL – end-of-life

Getting more plastic into the system

Research question: Which household interventions could most effectively increase collection rate of PET?

Approach: Agent-based model that simulates the trashing, recycling, and wish-cycling behavior of agents based on certain attributes.

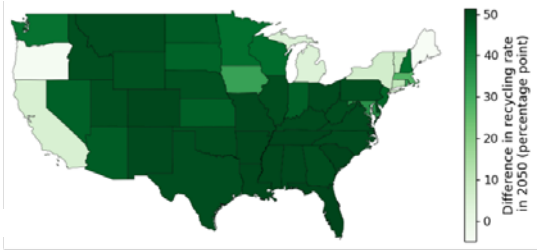


J. Walzberg *et al.*, *Energy Res. Soc. Sci.*, 2023, *100*, 103116

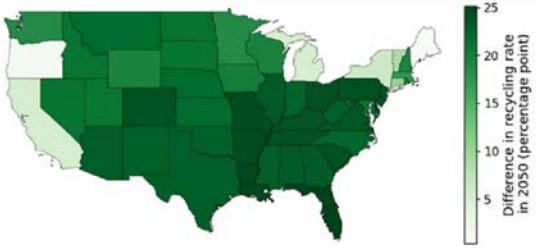
Getting more plastic into the system

- Various interventions could increase the U.S. average PET collection rate from 25% by up to 13-41 percentage points, depending on the state.
- Implementation would require ~$8.5-13/household but overall could reduce emissions from virgin plastic production by 0.5-0.7 MMT CO_2.

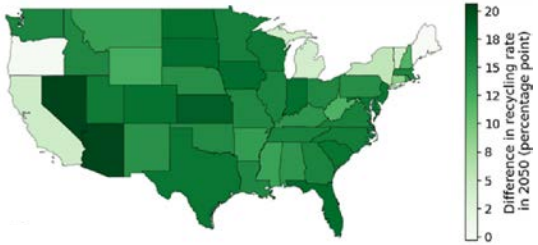
Expand deposit-return schemes



Improve education



Enable equitable recycling access



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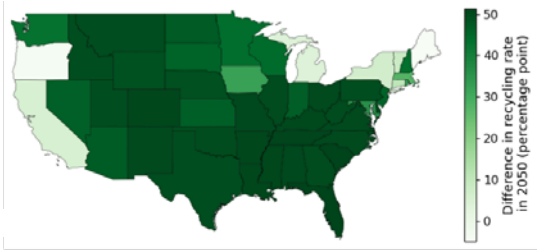
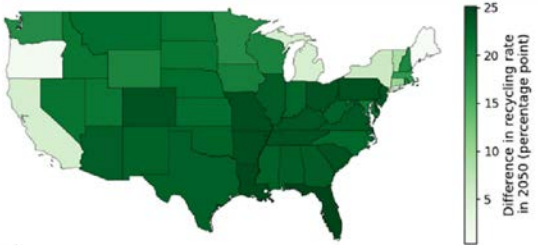
Getting more plastic into the system

- Various interventions could increase the U.S. average PET collection rate from 25% by up to 13-41 percentage points, depending on the state.
- Implementation would require ~$8.5-13/household but overall could reduce GHG emissions from virgin plastic production by 0.5-0.7 MMT CO_2.
- Some interventions could also decrease contamination from a U.S. average of 21% by up to 10-13 percentage points, depending on the state.

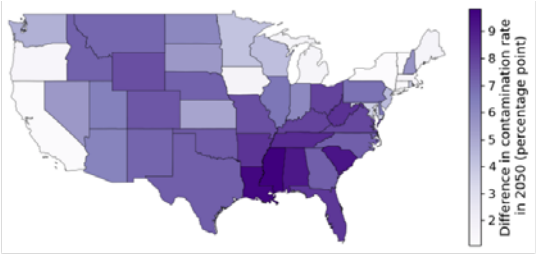
Expand deposit-return schemes



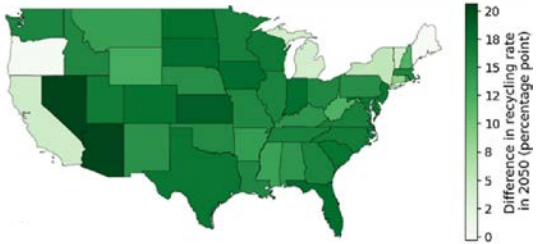
Improve education



Implement cart-tagging



Enable equitable recycling access



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Summary

The impact of analysis

Inform

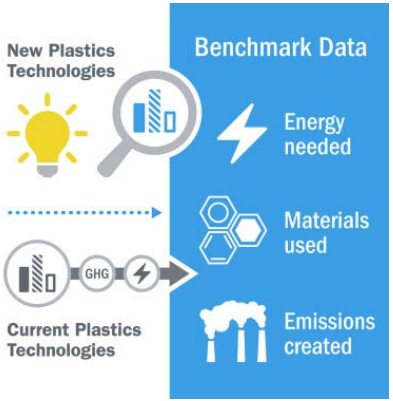
- Rigorous, consistent process modeling, TEA, LCA, and MFA.
- Serve the research community and industry.
- Work in open-access outlets with fully transparent data.

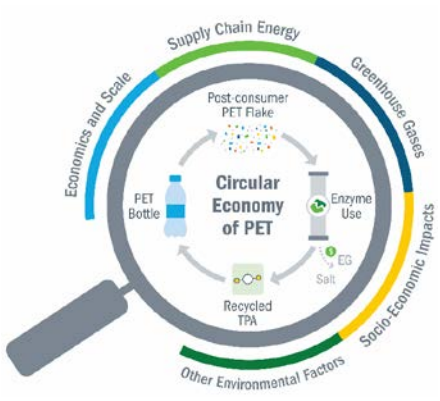
Guide

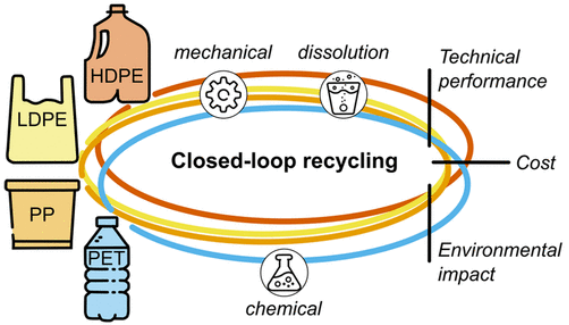
- Compare results against incumbent technologies.
- Highlight research gaps and opportunities for improvement.
- Use to off-board and on-board research directions.

Enable

- Facilitate decision-making and deployment of technologies for the plastics economy.







Figures sourced from (left to right): S.R. Nicholson, N.A. Rorrer *et al*. *Joule* 2021; A. Singh *et al*. *Joule* 2021.; T. Uekert *et al*. *ACS Sustain. Chem. Eng.* 2023.

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Thank you!

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