A Primer on Using Analysis to Guide Plastic Circularity

October 16, 2024

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https://www.bottle.org/

U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY
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bottle
changing the way we recycle
U.S. DEPARTMENT OF ENERGY

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Today's Speaker

Dr. Taylor Uekert
BOTTLE Analysis Co-Lead
taylor.uekert@nrel.gov

BOTTLE mission and goals

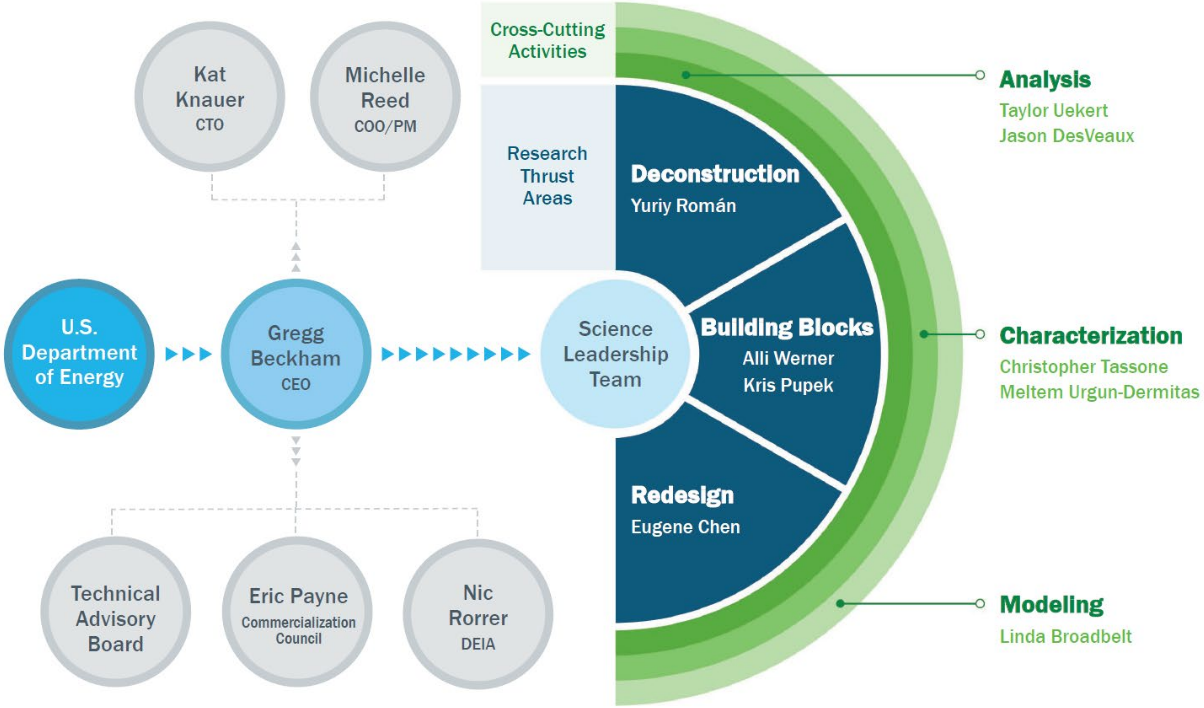
Mission

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

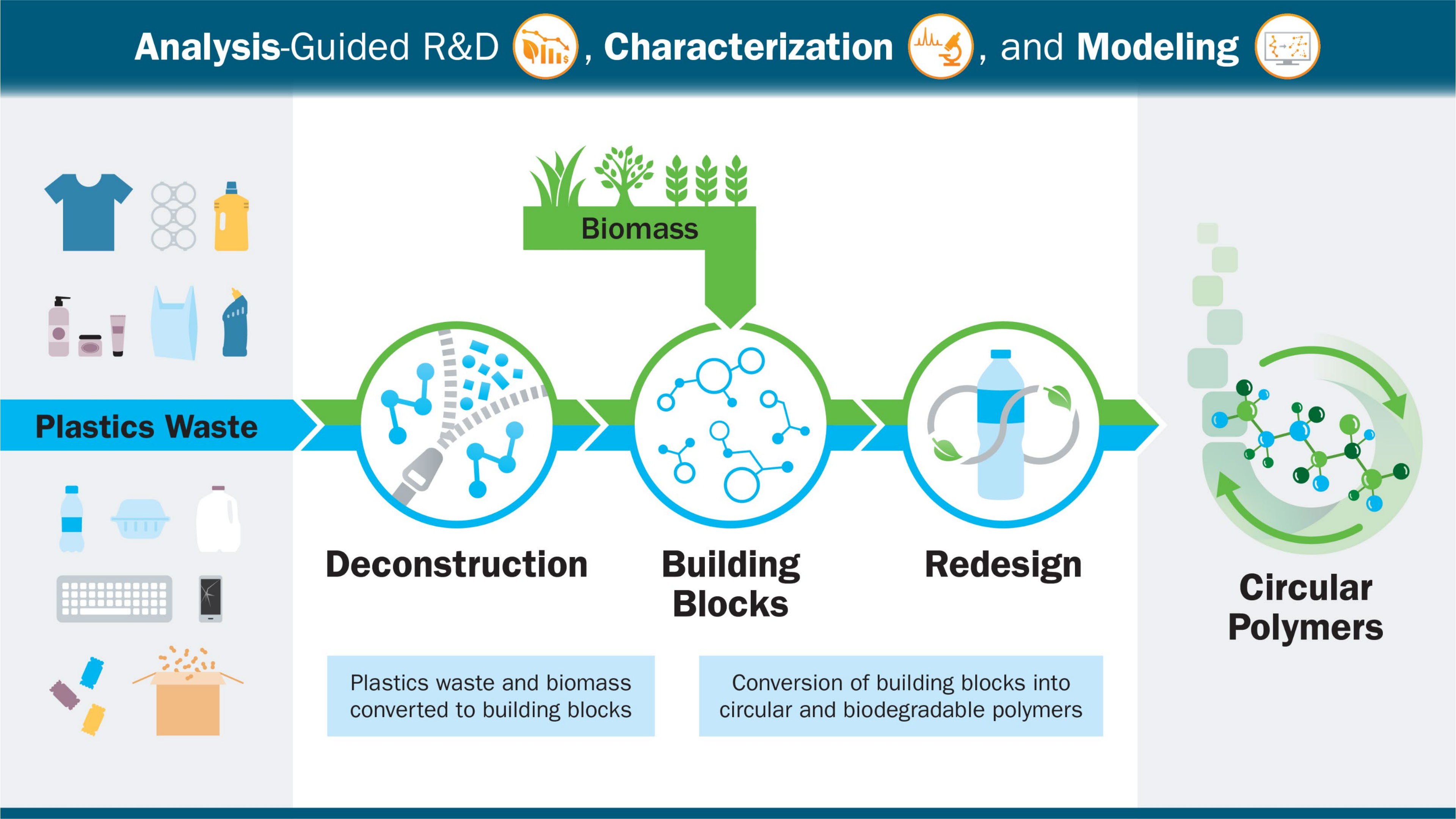
Goals

- Develop scalable, cost-effective processes to recycle plastics discarded in large quantities today.
- Design new bio-based chemistries and processes for manufacturing and recycling of circular plastics.
- Work with industry to catalyze a new circular paradigm for plastics.
- Foster a diverse and inclusive consortium.

BOTTLE Team & Structure



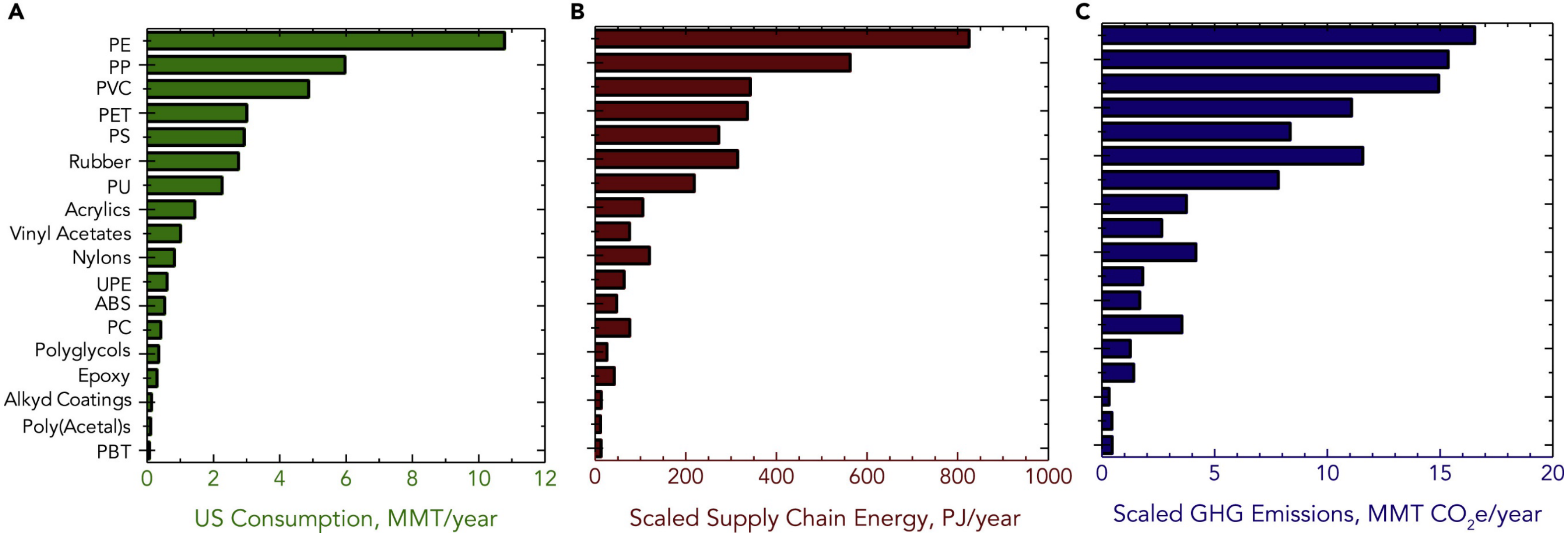
BOTTLE: Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment



Analysis-Guided R&D, Characterization, and Modeling
Biomass
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?

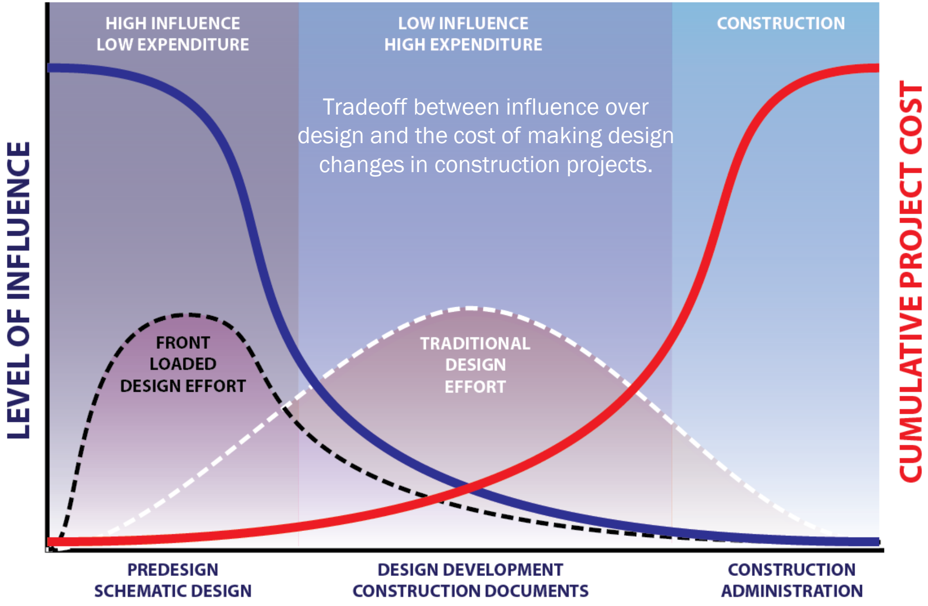
- Plastic production and disposal in the U.S. today have known implications: 2% of total U.S. greenhouse gas (GHG) emissions and 44 million metric tons (MMT) of landfilled or incinerated waste.
- A circular economy could reduce waste *and* the impacts associated with virgin plastic production.



S. R. Nicholson, et al., *Joule*, 2021, *5*, 673-686; A. Milbrandt et al., *Resourc. Conserv. Recycl.*, 2022, *183*, 106363.

Why analysis-guided R&D?

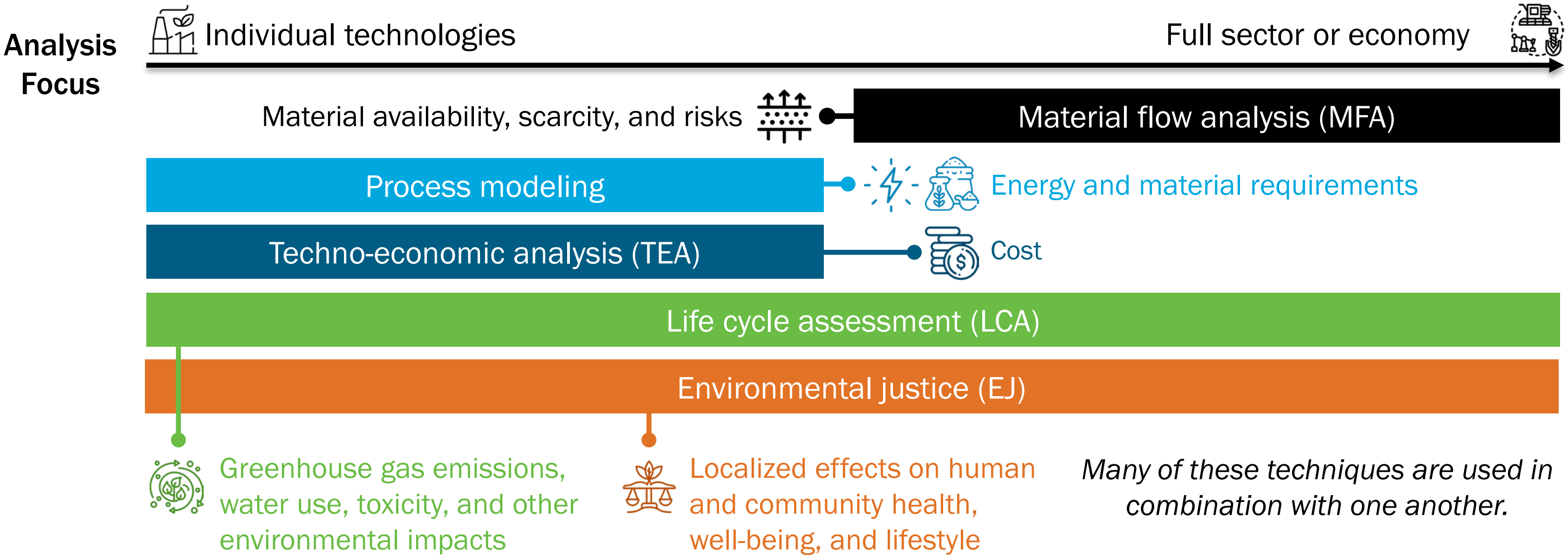
- As we design a circular future, innovations should mitigate harms rather than causing more.
- Negative impacts can be “locked in” by early-stage R&D decisions. More opportunities exist to address impacts the earlier they are considered.



Wheeler Kearns Architects; Paulson, 1976

Analysis methods

Types of analysis

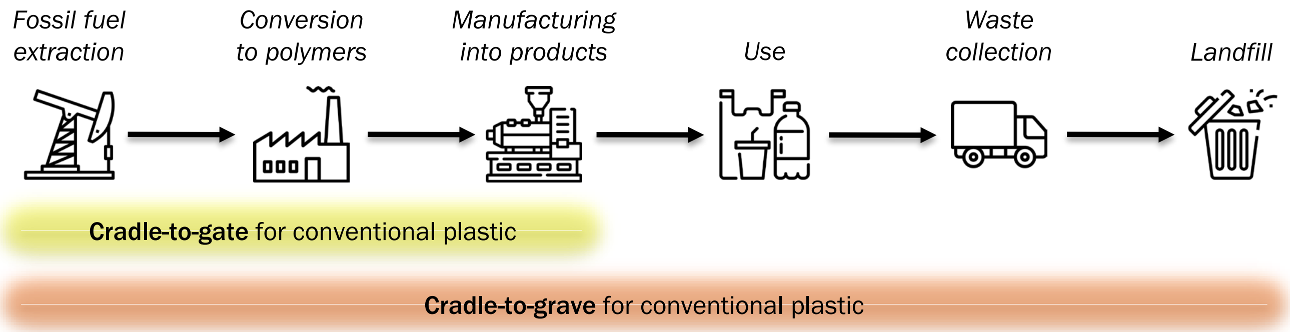


Many of these techniques are used in combination with one another.

* Key vocabulary will be bolded in the following slides.

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?



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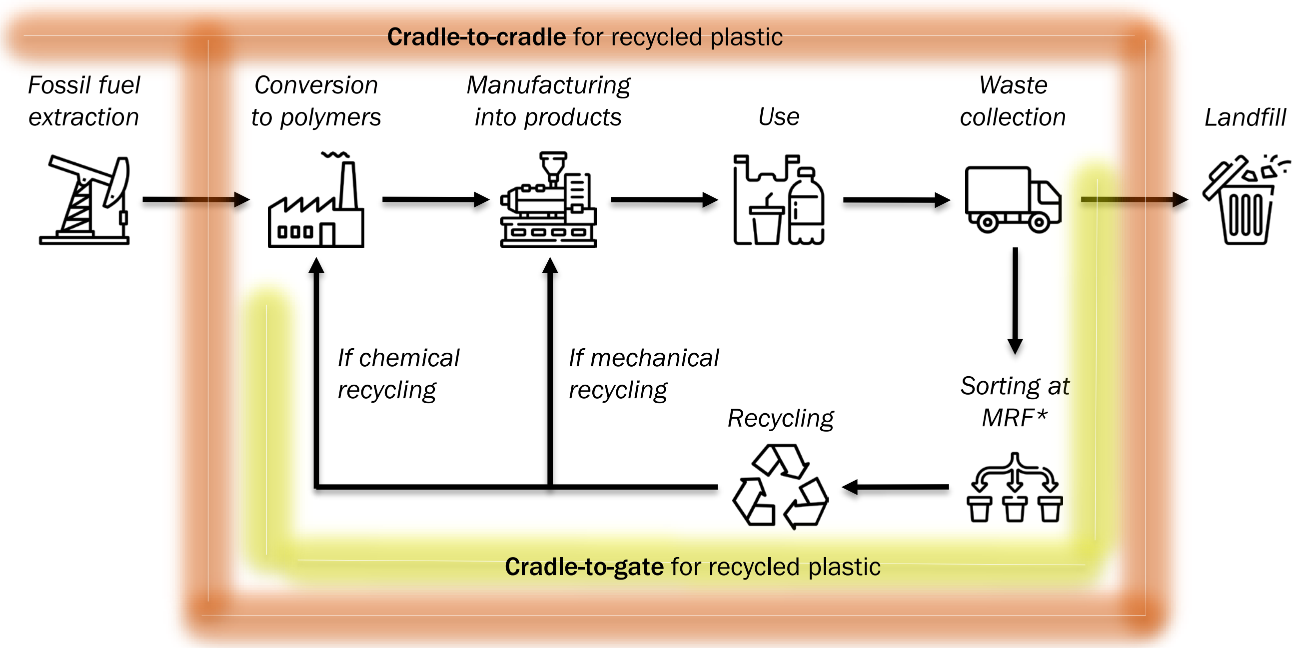
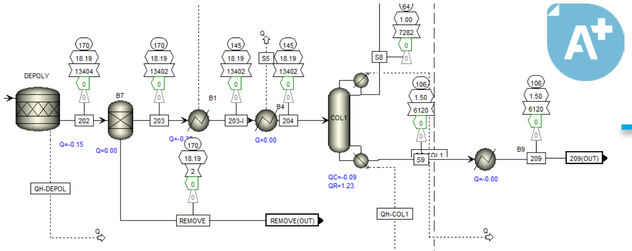


* MRF = materials recovery facility

Analysis methods

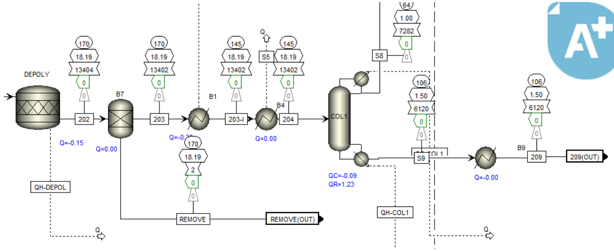
Collect data & build process model



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

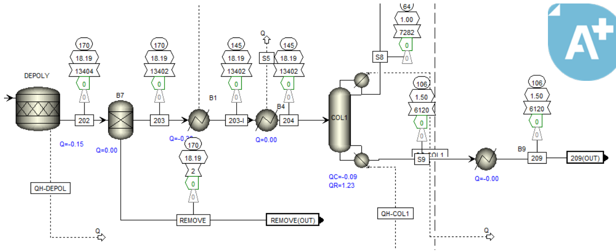
- Use prices from proprietary databases to calculate **operational expenses** (**OPEX**) and Aspen estimates or company quotes to determine **capital expenses (CAPEX).**
- Calculate **minimum selling price** (**MSP**) in $/kg.

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
Other Variable Costs				$33,700,857	$38,515,265	$38,515,26
Fixed Operating Costs				$5,277,349	$5,277,349	$5,277,34
Total Product Cost				$51,912,894	$61,038,864	$61,038,86
Annual Depreciation						
General Plant Writedown				14%	24.49%	17.49%
Depreciation Charge				$18,455,190	$31,628,243	$22,587,91
Remaining Value				$110,692,394	$79,064,150	$56,476,23
Steam Plant Writedown				3.75%	7.22%	6.68%
Depreciation Charge				$540,731	$1,040,942	$962,78
Remaining Value				$13,878,750	$12,837,808	$11,875,01
Net Revenue				($16,410,748)	($18,549,681)	($8,969,043
Losses Forward					($16,410,748)	($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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LCA

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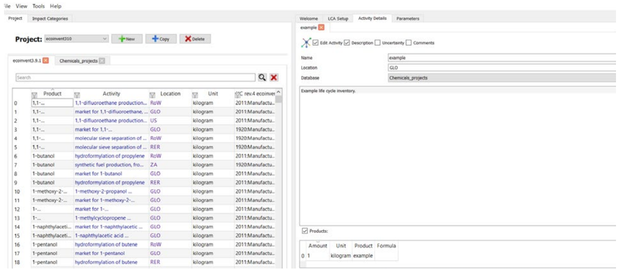
Impact assessment

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



Analysis methods

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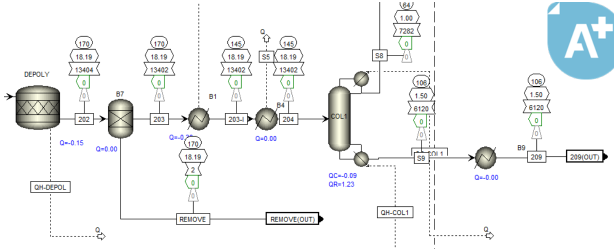

Material and energy flows (aka **life cycle inventory** or **foreground data**)

EJ

Qualitative analysis

- Explore local community and worker safety impacts.

TEA

LCA

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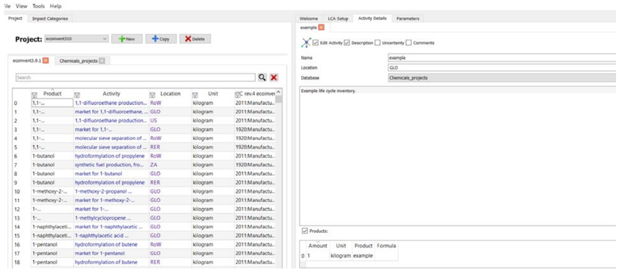


Filling data gaps

Imagine our process uses or produces a new material, like a complex catalyst, solvent, or monomer mixture.

Process modeling

Problem: missing thermodynamic properties

Solutions: literature search, experimental validation, proxy assumptions

TEA

Problem: unknown cost

Solutions: tools such as CatCost, 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

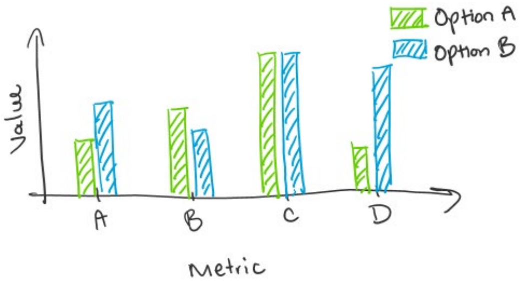
Analysis interpretation

Interpret results:

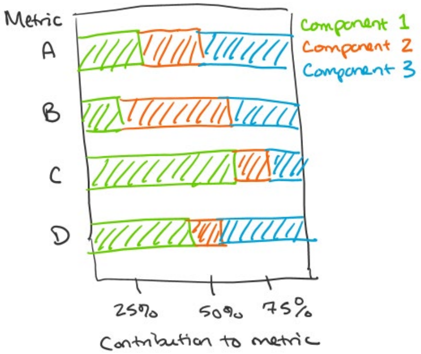
- Comparison – how does the new process compare to conventional?
- Hotspots – which materials or energy are the biggest contributors to each metric?
- Sensitivity – how big of an affect will changing key parameters have?
- Uncertainty – how reliable are your results?
- Multi criteria decision analysis (MCDA) – what is the overall "score" across multiple metrics to enable decision-making in the face of tradeoffs?

Iterate:

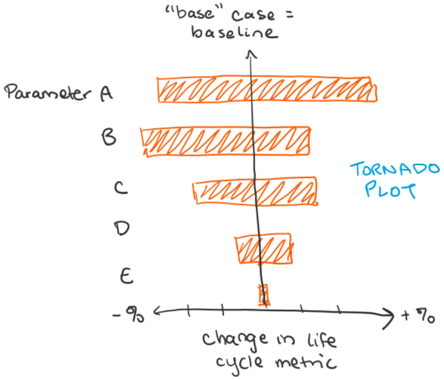
- Adapt process and model to address problem areas
- Communicate opportunities for improvement



Comparison



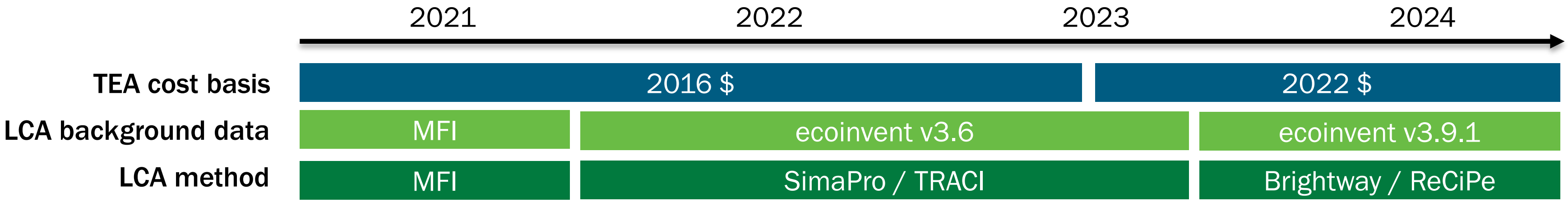
Hotspots



Sensitivity

Caveats

- We strive for consistency and transparency in all our analyses.
- But analysis is not static! We also update our methods and data periodically.
- The BOTTLE analysis approach is not everyone’s analysis approach. Take the time to understand the assumptions behind any published work.



A cautionary tale of two analyses

Two LCAs of plastic pyrolysis → one showed higher impacts of pyrolysis than fossil products, and the other showed equivalent impacts of pyrolysis and fossil products. Why are they different?

A cautionary tale of two analyses

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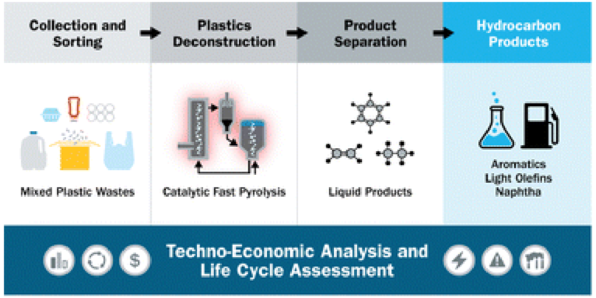
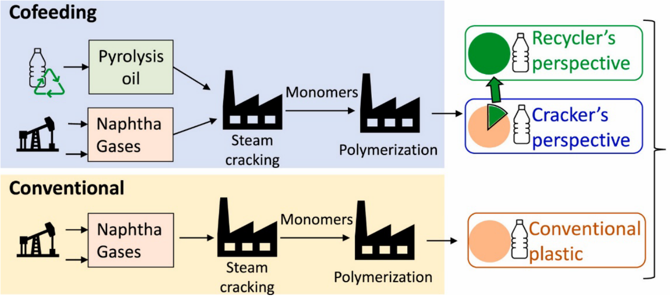
Data source:	Open-access literature and patents	Company surveys
Feedstock:	Post-consumer polyolefins	Post-consumer and post-industrial polyolefins
Target product:	*Direct* products from pyrolysis (naptha, benzene-toluene-xylene, or ethylene)	Polyethylene from *co-feeding* 5-20% pyrolysis oil into an existing fossil-based plant
Applied credits:	Co-products only	Fossil naphtha production “avoided” by pyrolysis





(Left) G. Yadav et al., *Energy Environ Sci.*, 2023, *16*, 3638-3653. (Right) U. R. Gracida-Alvarez et al., *J. Clean. Prod.*, 2023, *425*, 138867

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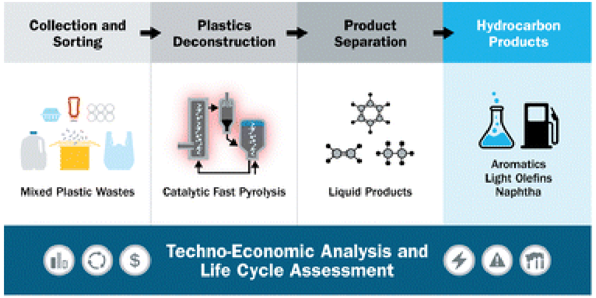
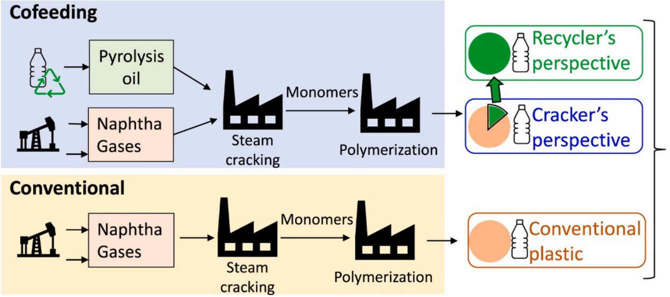




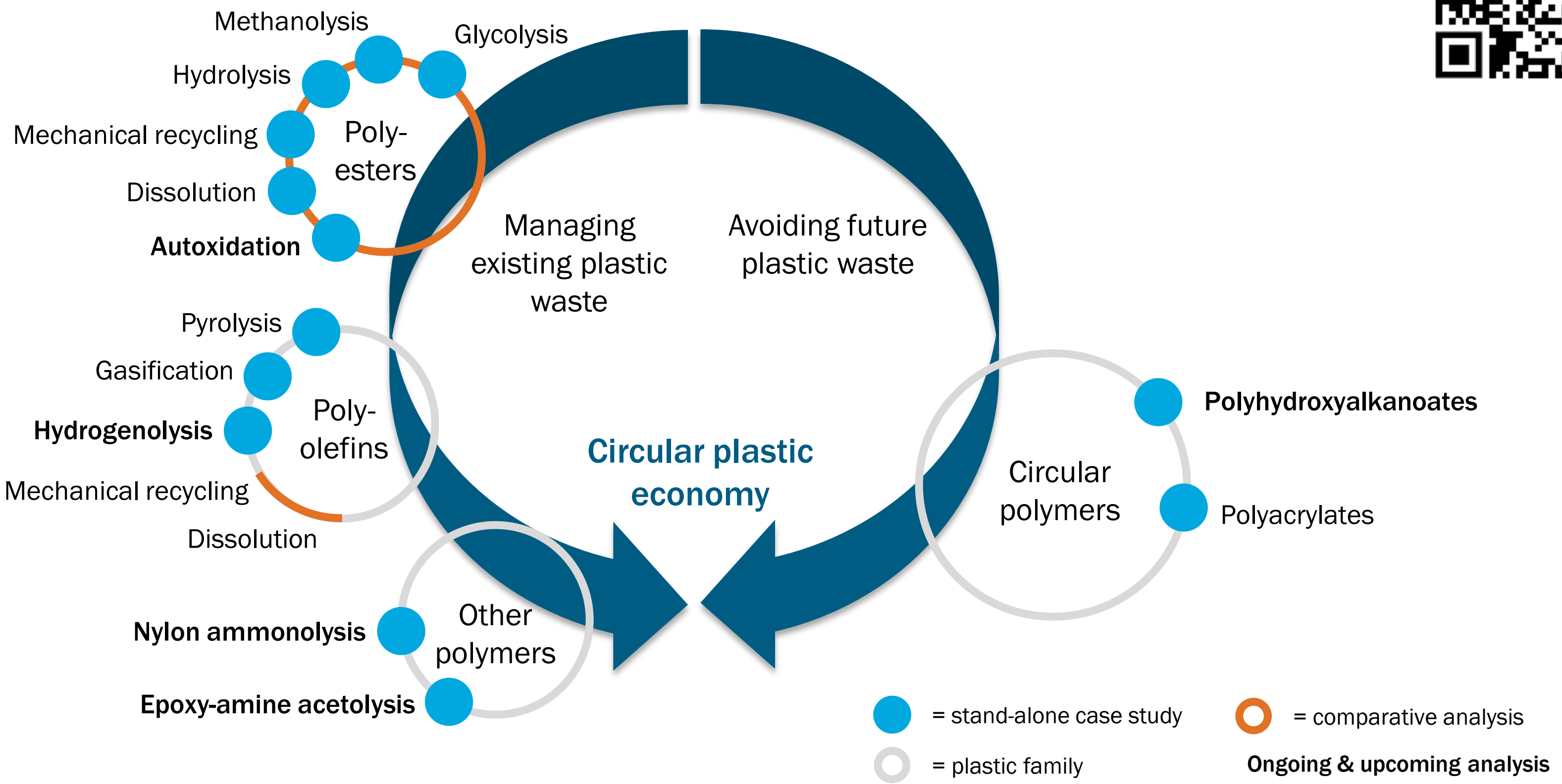
Check assumptions before deciding if an analysis is applicable to your work.

(Left) G. Yadav et al., *Energy Environ Sci.*, 2023, *16*, 3638-3653. (Right) U. R. Gracida-Alvarez et al., *J. Clean. Prod.*, 2023, *425*, 138867

Analysis examples

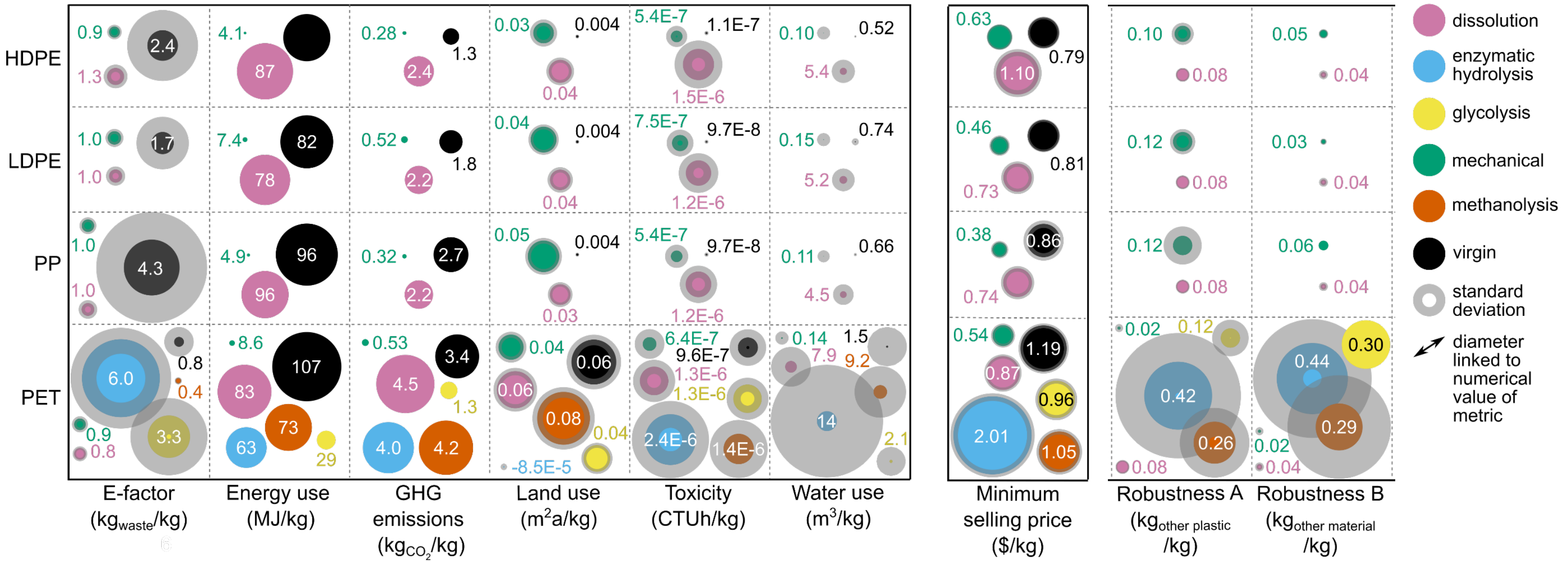
Overview of analysis studies

https://www.bottle.org/research/analysis



Example 1: Comparing technologies

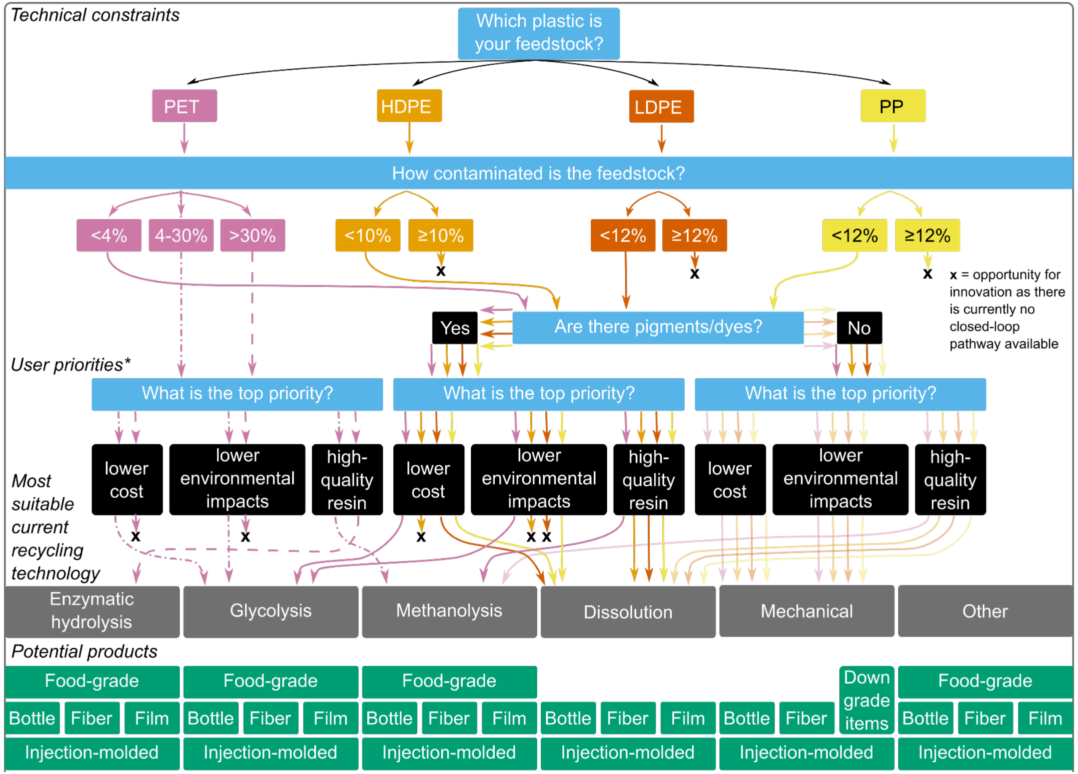
- Most relevant for: researchers trying to contextualize their work, decision-makers.
- How do mechanical and chemical recycling strategies for plastics compare across environmental, economic, and technical parameters?



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

Example 1: Comparing technologies

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



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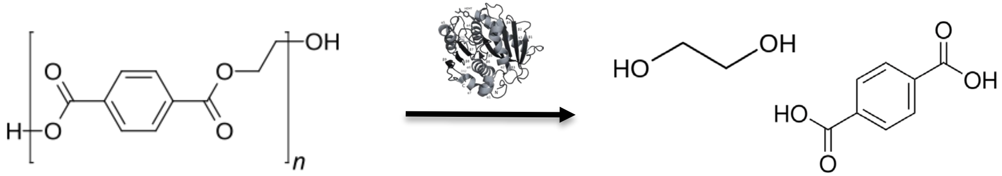
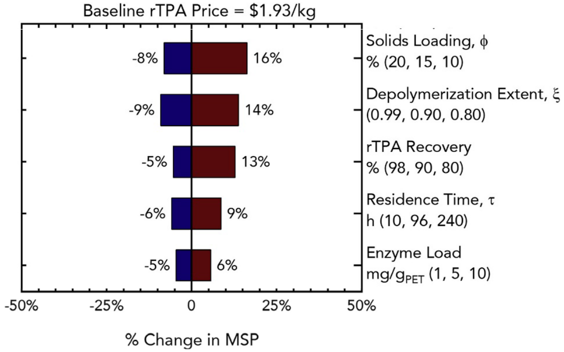
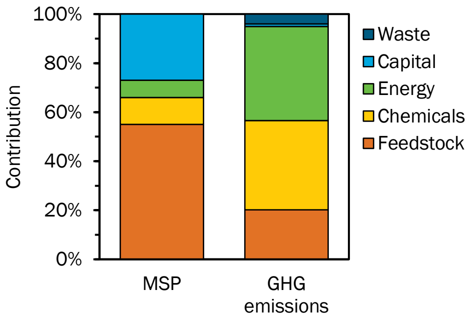
Example 2: Optimizing a technology

- Most relevant for: researchers or companies targeting maximal improvement of their technology.
- What are the key driving factors of enzymatic recycling of poly(ethylene terephthalate) (PET) bottles?



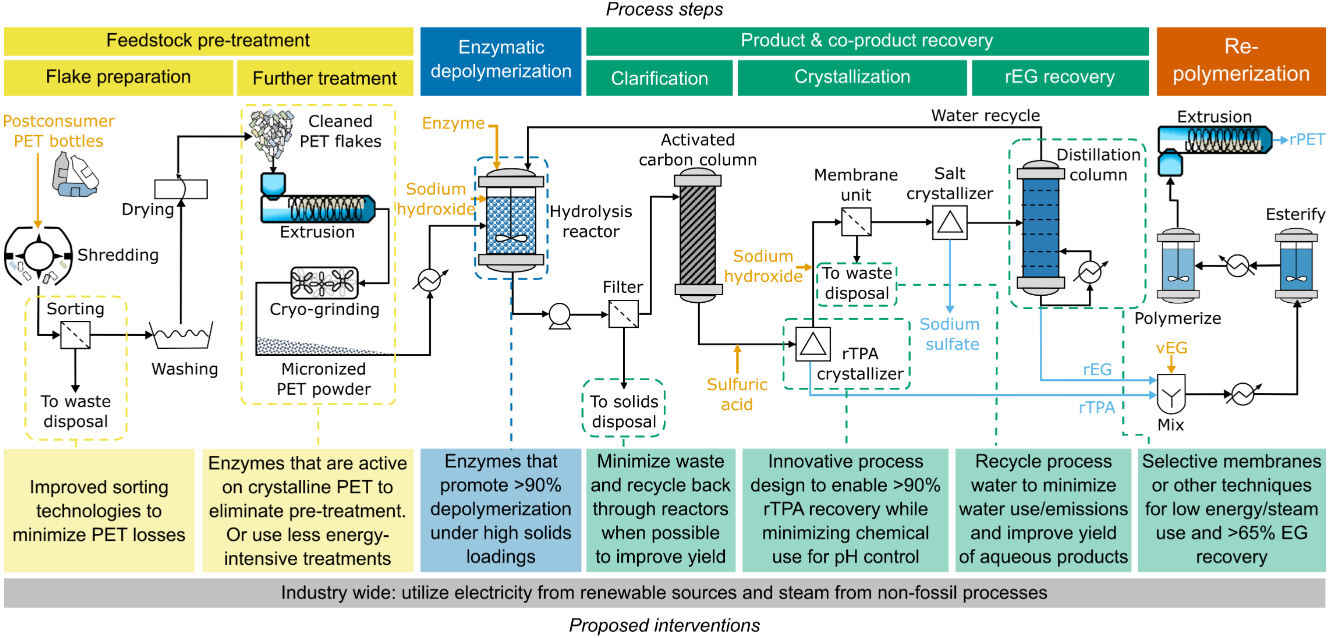


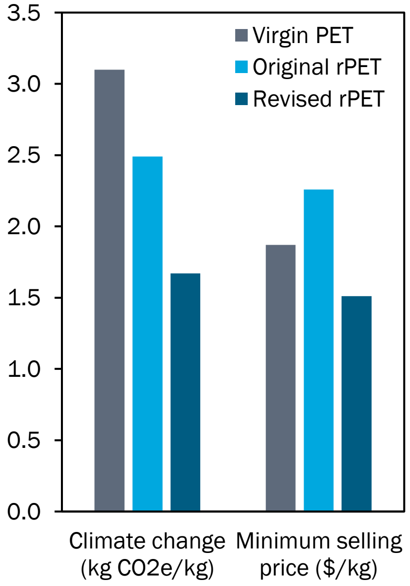


A. Singh et al., *Joule,* 2021, *5*, 2479-2503. T. Uekert et al., *Green Chem.,* 2022, 24, 6531.

Example 2: Optimizing a technology

Return to the lab and process model to determine how to maximize yield, minimize waste pre-treatment, and minimize sodium hydroxide use. → Revised process shows marked improvement.





(Left) T. Uekert et al., *Green Chem.*, 2022, *24*, 6531. (Right) N. Murphy, S. Dempsey & J. DesVeaux, et al., *submitted.*

Example 2: Optimizing a technology

This iterative process also enables improvement to the EJ outcomes of enzymatic recycling:

Problem	Action	Effect
Toxic materials Sulfuric acid for terephthalic acid recovery	*Switch to ammonia*	Ammonia is still toxic but can be recovered and so **used in lower quantities** (0.02 kg/kg PET vs. 0.6 kg sulfuric acid / kg PET).
Hazardous waste Ethylene glycol to waste-water; unreacted solid waste	*Recycle the reaction solution*	Yield increases, **halving solid waste** generation and **reducing ethylene glycol** emissions by 15%.
End-of-life Only if PET returns to recycling process	*Maximize yield*	Maximize the amount of PET that could in theory be **recycled again.**

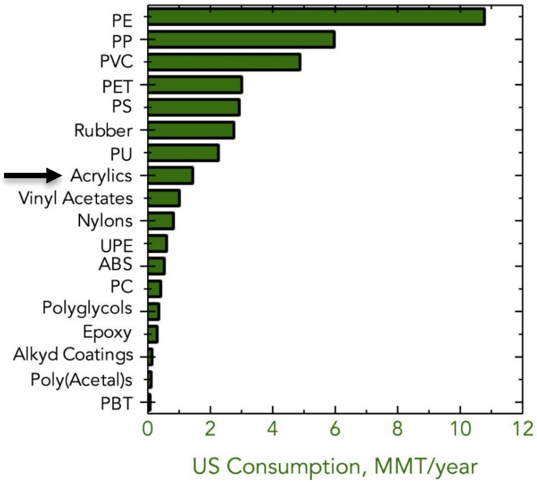
Want to learn how to do an EJ analysis?

Register Interest in Energy & Environmental Justice Training

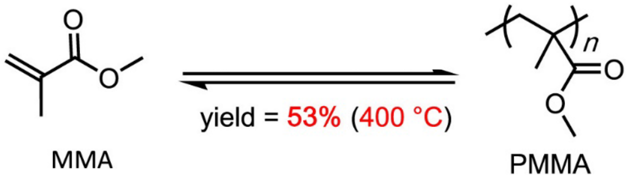
T. Uekert et al., *ACS Sustain. Chem. Eng.*, 2024, *12*, 8307; N. Murphy et al., *submitted*

Example 3: Circularity in analysis

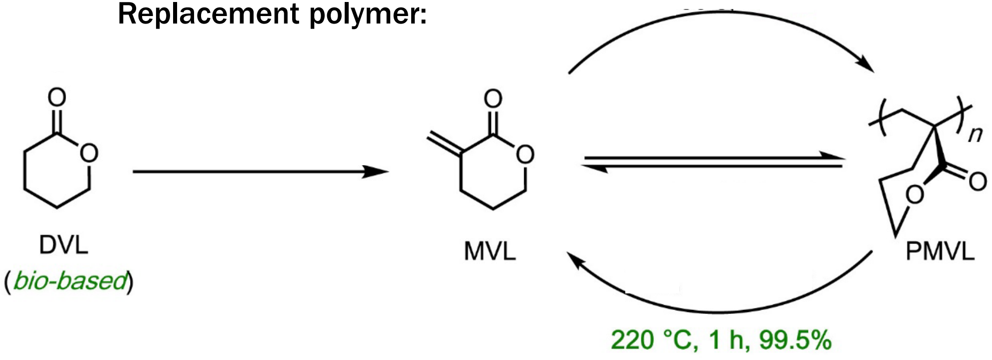
- Most relevant for: researchers.
- Bio-based poly(α-methylene-δ-valerolactone) (PMVL) exhibits properties similar to poly(methyl methacrylate) (PMMA), but with inherent chemical recyclability.



Current polymer:



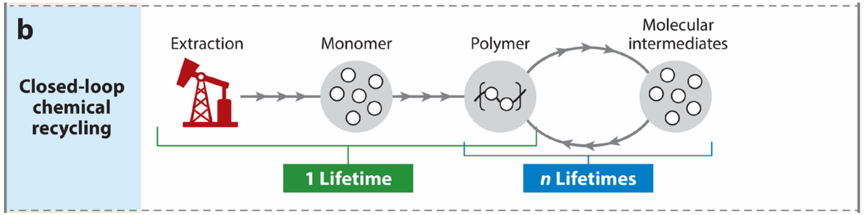
Replacement polymer:



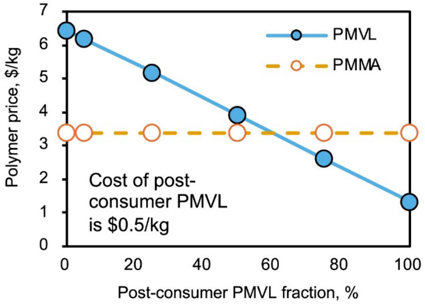
R. A. Gilsdorf, et al., *Cell Rep. Phy. Sci.*, 2024, *5*, 101938.

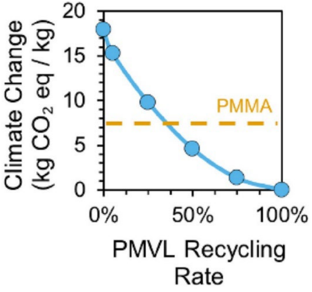
Example 3: Circularity in analysis

Exploring the effect of multiple lifetimes on TEA and LCA shows that a 50-60% recycling rate could enable PMVL to economically and environmentally compete with PMMA.



Use yields to estimate # of product lifetimes. Normalize impacts across lifetimes.





(Left) S. R. Nicholson et al., *Ann. Rev. Chem. Biomolec. Eng.*, 2022, *13*, 301. (Right) R. A. Gilsdorf et al., *Cell Rep. Phy. Sci.*, 2024, *5*, 101938.

Summary

The impact of analysis

Inform

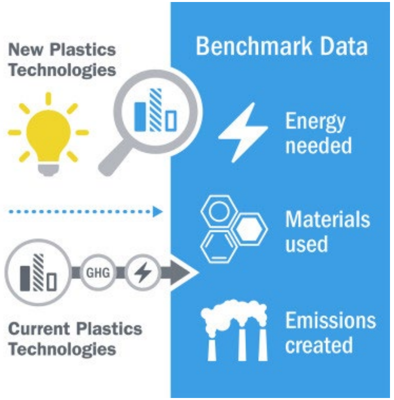
- Rigorous, consistent process modeling, TEA, LCA, and EJ.
- Serve the research community and industry.
- Work in open-access outlets with fully transparent data.

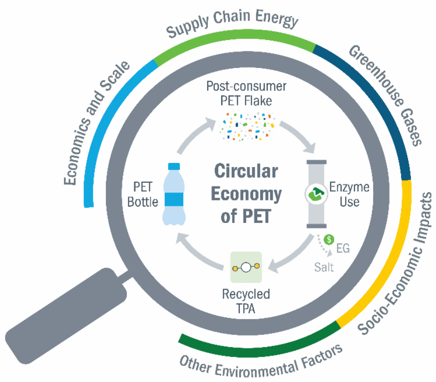
Guide

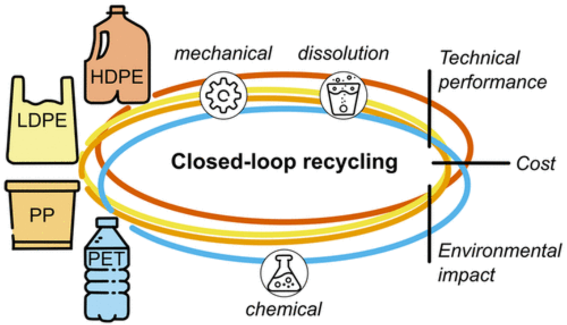
- Compare results against incumbent technologies.
- Highlight research gaps and opportunities for improvement.
- Use to off-board and on-board research directions.

Enable

- Facilitate deployment of technologies for a more circular, sustainable plastics economy.
- Work with researchers to improve processes before first experimental reports appear.







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.

Read the literature (critically)

Try your own preliminary analysis

Collaborate with experts

Incorporate learnings into experimental process

Think holistically

Incorporate analysis into your own work

Analysis team

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Postdoctoral TEA researcher

Birdie Carpenter
Platform lead

Elisabeth Van Roijen
Postdoctoral LCA researcher

Geetanjali Yadav
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Rarosue Amaraibi
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Thank you!

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This work was authored by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Advanced Materials Technologies Office and Bioenergy Technologies Office. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.