bottle
changing the way we recycle
U.S. DEPARTMENT OF ENERGY

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

DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

BOTTLE 2 – Analysis

April 3, 2023

Technology Session Review Area: Plastics Deconstruction and Redesign

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Presenters: Gregg T. Beckham, Jason DesVeaux, and Taylor Uekert, National Renewable Energy Laboratory

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BIOENERGY TECHNOLOGIES OFFICE
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Overview: Analysis and its role in BOTTLE

Analysis is foundational to BOTTLE's mission

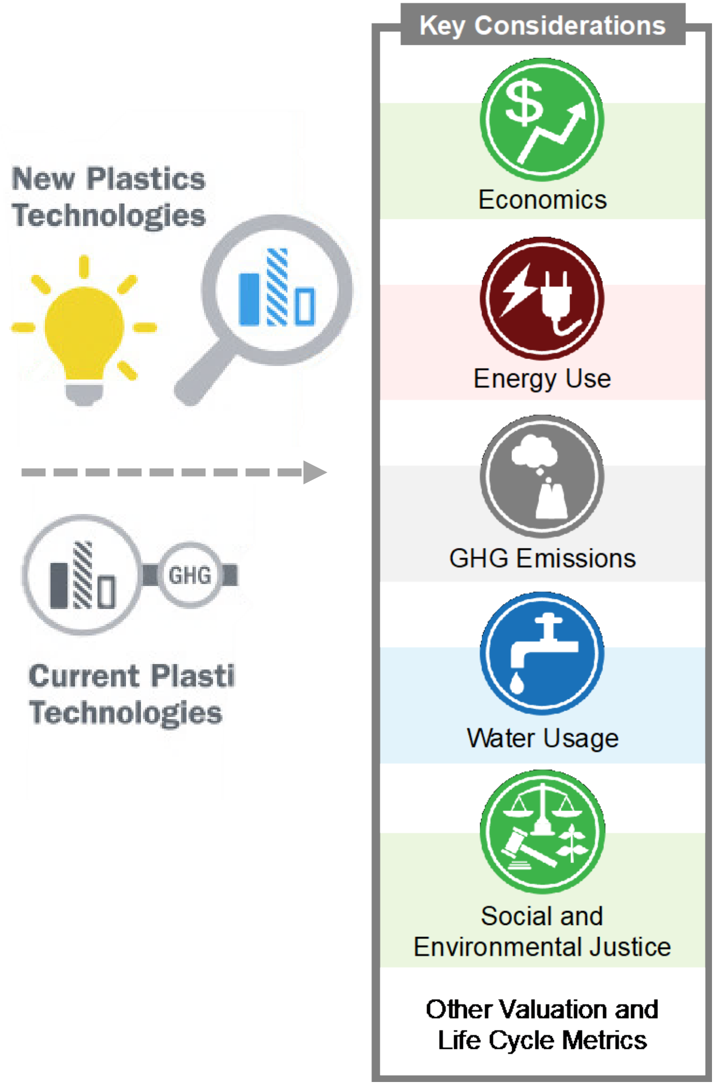
- Develop robust processes to upcycle existing waste plastics, and
- Develop new plastics and processes that are recyclable-by-design
- Analysis-guided R&D aligns with DOE's Strategy for Plastics Innovation

Economic, environmental, and comparative analysis

- Model new processes and analyze energy, carbon, cost, and GHG emissions metrics to determine their feasibility and key driving variables
- Compare these results against incumbent technologies

Framework for analysis proposed in 2022 review[1]

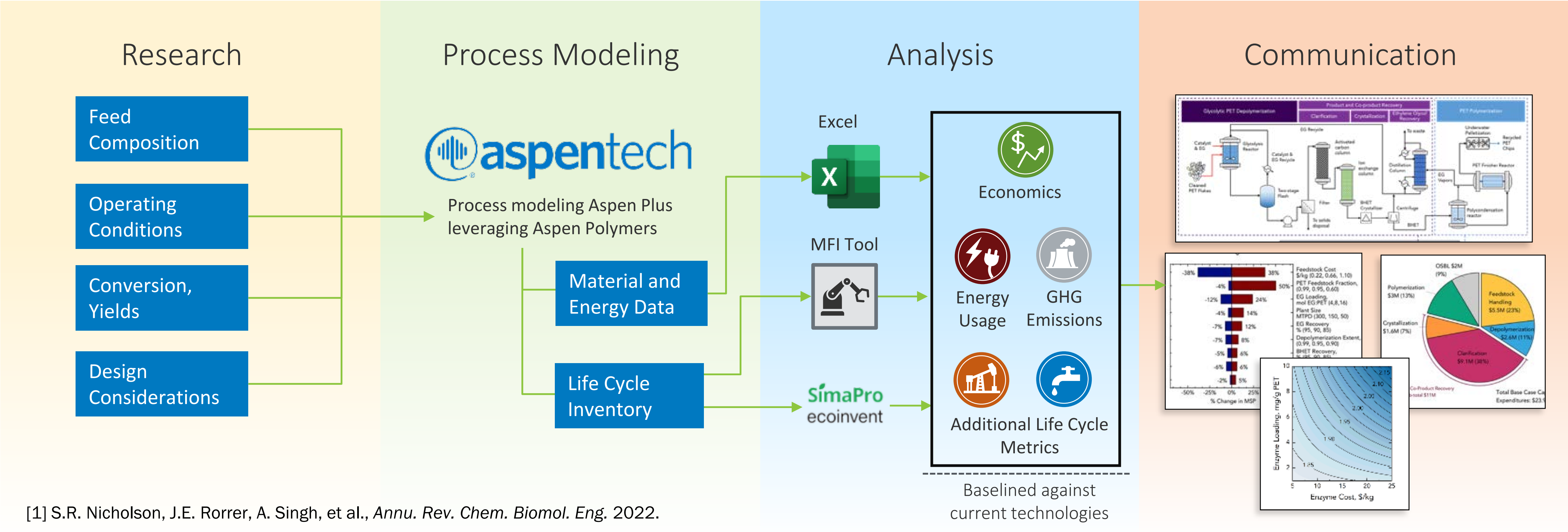
- Identify impactful areas for R&D
- Guide technologies towards a circular and sustainable plastics economy



[1] S.R. Nicholson, J.E. Rorrer, A. Singh, et al., *Annu. Rev. Chem. Biomol. Eng.* 2022. Image sourced from reference at left and S.R. Nicholson, N.A. Rorrer et al., *Joule* 2021.

Analysis approach

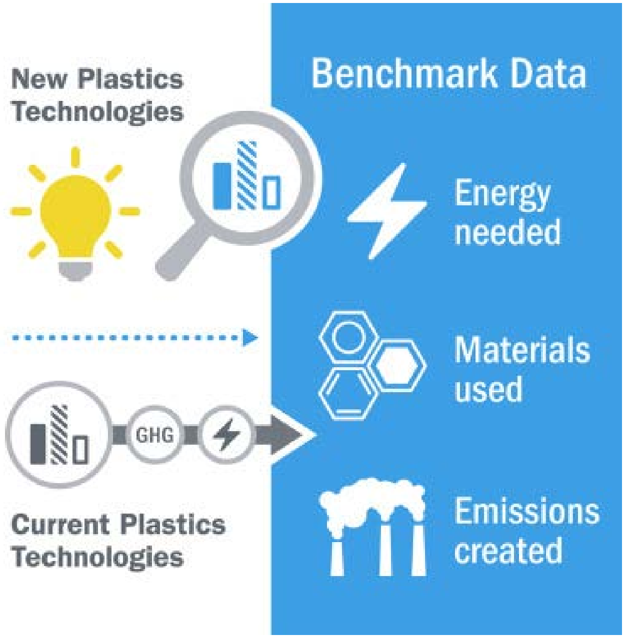
- Techno-economic analysis (TEA) and life-cycle assessment (LCA) conducted across multiple scopes
- Economics and sustainability assumptions follow transparent / open-source practices in EERE-funded R&D; framework published in recent review[1]
- Analysis is an iterative process that occurs in parallel to laboratory R&D
- Communication with each task through fortnightly team meetings and internal task meetings
- Select risks include data availability and ability to incorporate feedstock variability and quality into models

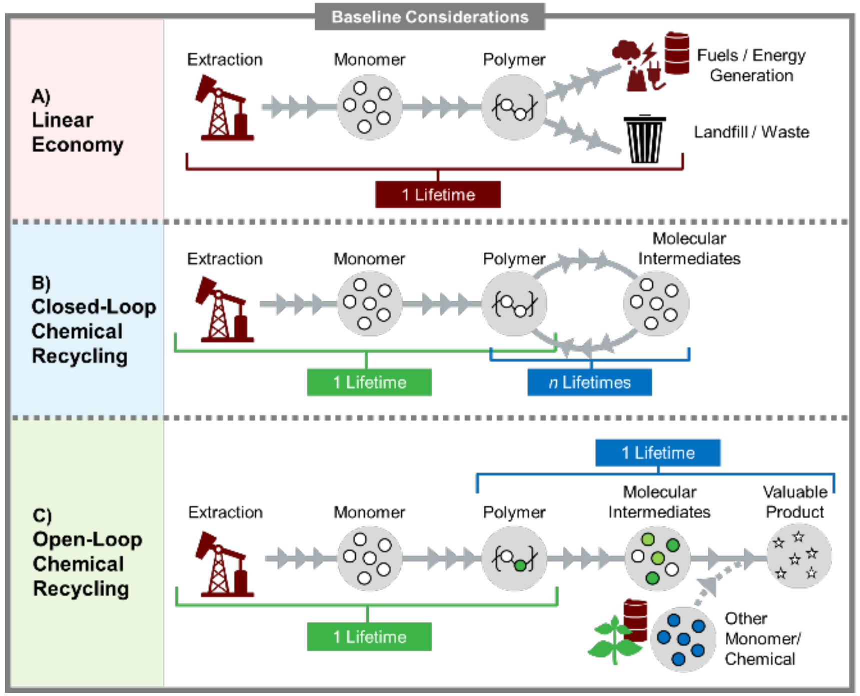


[1] S.R. Nicholson, J.E. Rorrer, A. Singh, et al., *Annu. Rev. Chem. Biomol. Eng.* 2022.

Outline of progress and outcomes

- Benchmarked metrics for virgin plastic production[1]
- Established analysis framework for evaluating recycling technologies[2]
- Evaluated new and existing plastic technologies





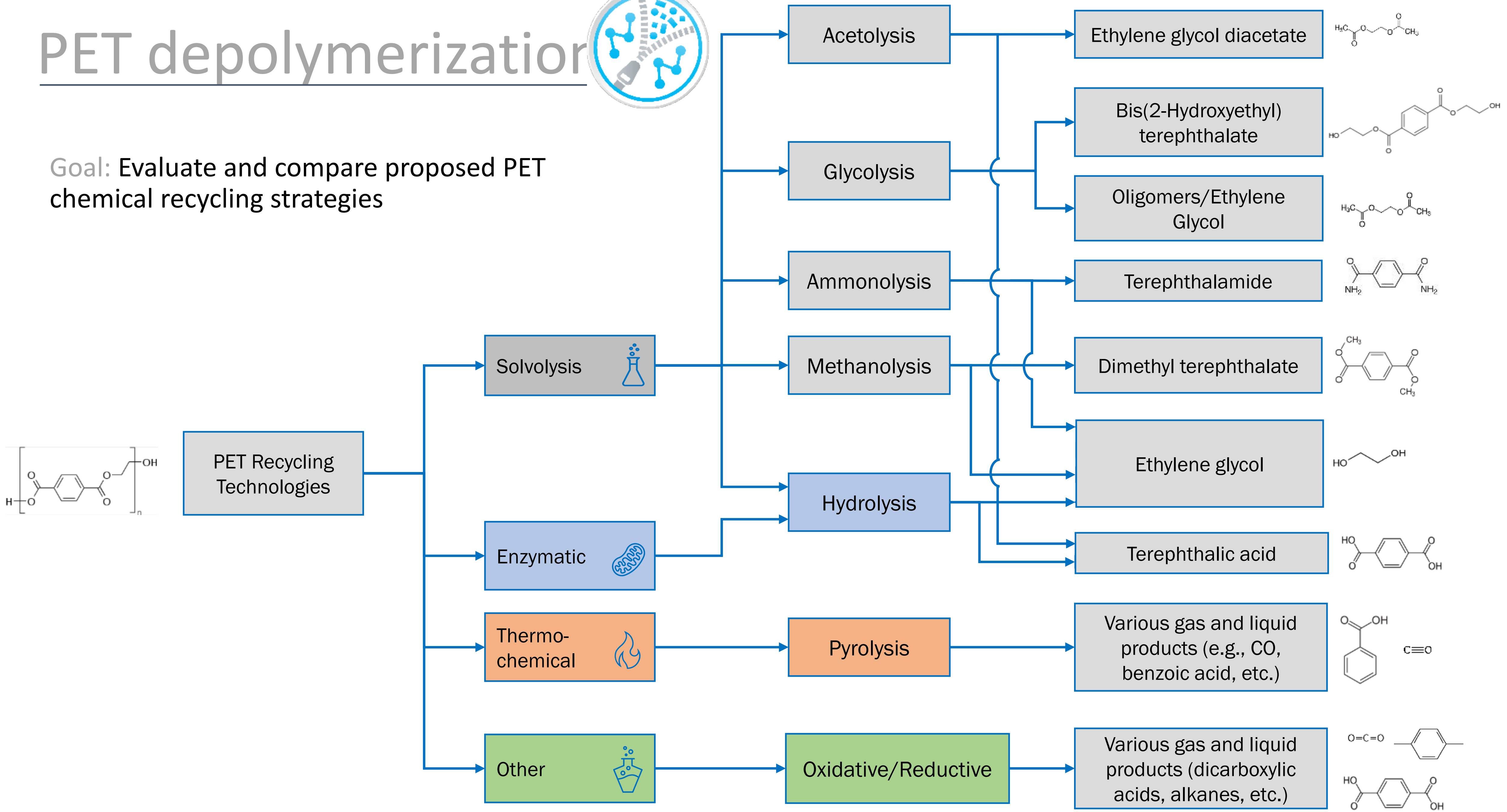
- ✓ Baseline analyses published or in peer review for:
  - ✓ PET deconstruction,[3-6]
  - ✓ Mixed plastic pyrolysis & gasification,[7-8]
  - ✓ Mechanical recycling[6]
- ❖ Additional recycling technologies in progress
- ❖ Redesign polymer pathways in progress

Focus of Today's Talk

[1] S.R. Nicholson, N.A. Rorrer *et al. Joule* 2021. [2] S.R. Nicholson, J.E. Rorrer, A. Singh *et al. Annu. Rev. Chem. Biomol. Eng.* 2022. [3] A. Singh *et al. Joule* 2021. [4] T. Uekert *et al. Green Chem.* 2022. [5] N.A. Rorrer *et al. in preparation* 2023. [6] T. Uekert *et al. ACS Sustain. Chem. Eng.* 2023. [7] G. Yadav *et al. in revision*. [8] S. Afzal *et al. in revision*.

PET depolymerization

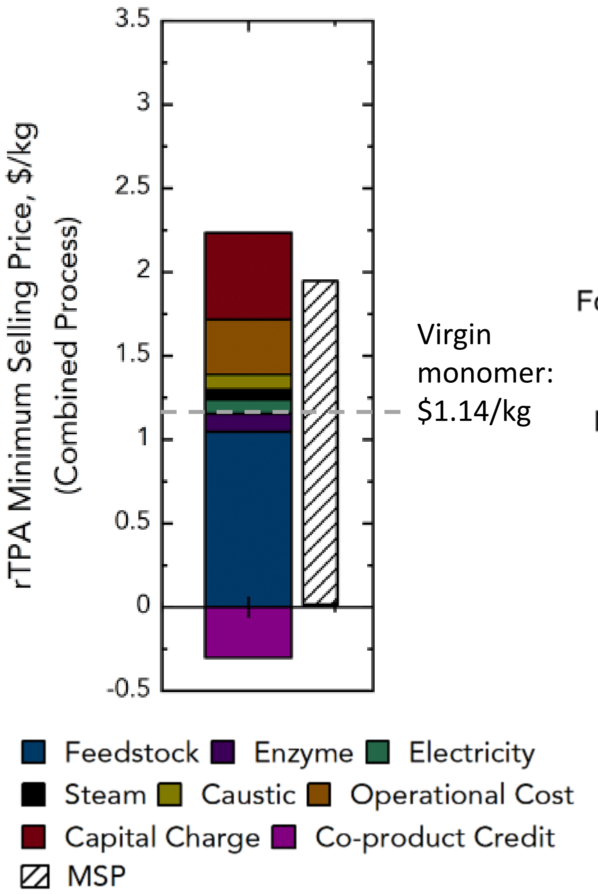
Goal: Evaluate and compare proposed PET chemical recycling strategies



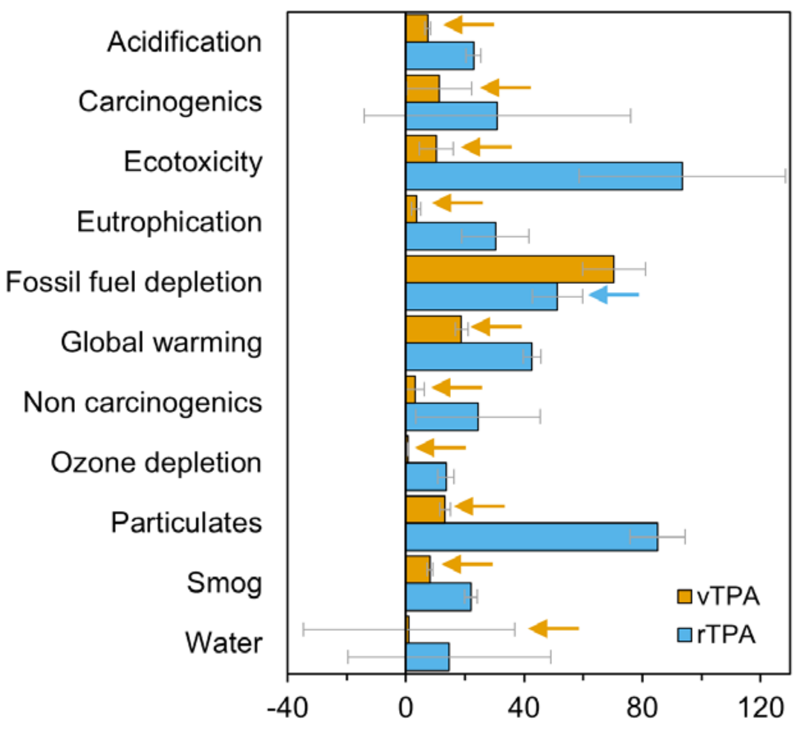
J. DesVeaux, T. Uekert, A. Singh, *et al.*, multiple papers published or in preparation

Case study I: PET enzymatic hydrolysis

Economic feasibility[1]



Environmental impact[2]

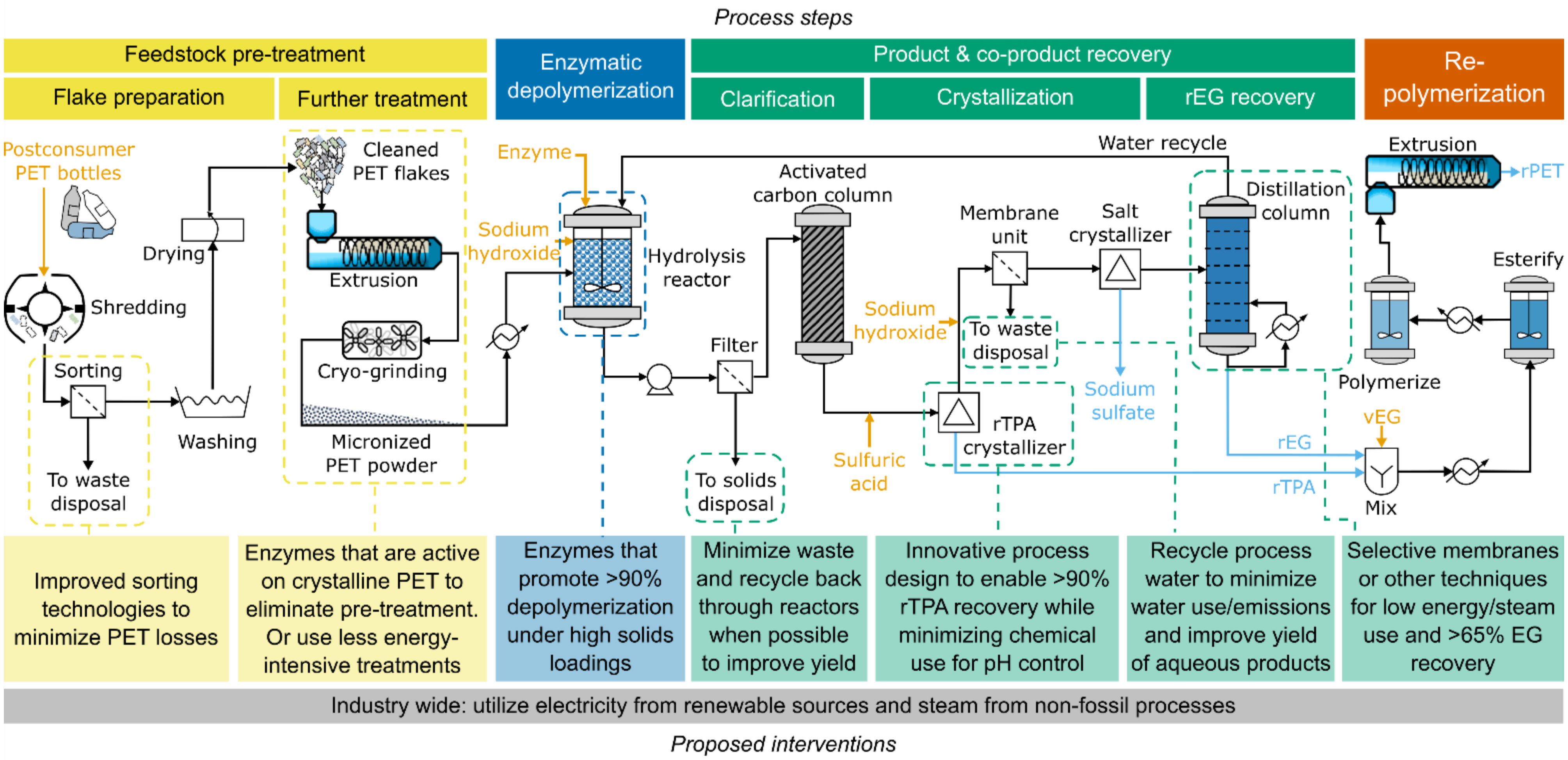


Goal: benchmark PET enzymatic recycling versus virgin PET manufacturing and identify areas for innovation

- Cost: Recycled terephthalic acid (rTPA) monomer is 1.7× more expensive than virgin vTPA
- Opportunity: Cheaper feedstock enables cost parity
- Environmental impact: rTPA has 3-17× higher impacts than vTPA (except fossil fuel depletion)
- Opportunity: New process designs reduce electricity and chemical use, enabling environmental parity

[1] A. Singh *et al. Joule* 2021 [2] T. Uekert *et al. Green Chem.* 2022

Research insights



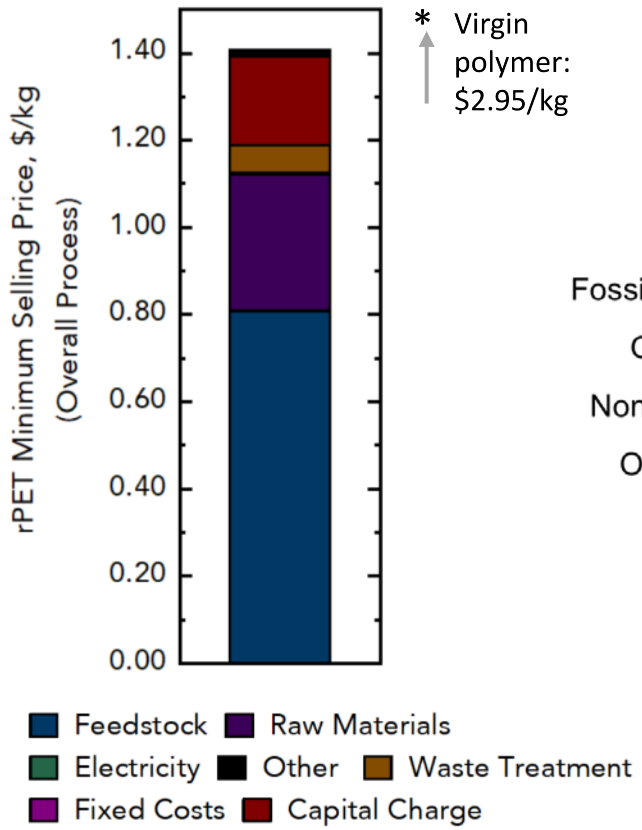
Improvements across many of these process areas will likely be necessary for scale-up of enzymatic recycling

Tradeoffs: many inexpensive components (water, steam, waste, etc.) are costly from an environmental perspective

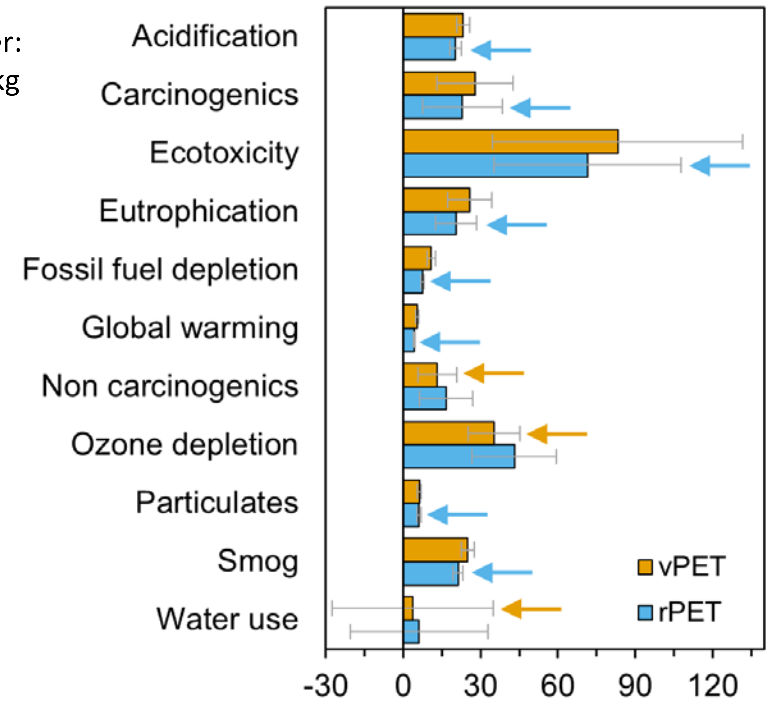
T. Uekert *et al. Green Chem.* 2022.

Case study II: PET glycolysis

Economic feasibility



Environmental impact



Goal: benchmark catalytic PET glycolysis against virgin PET and identify areas for innovation

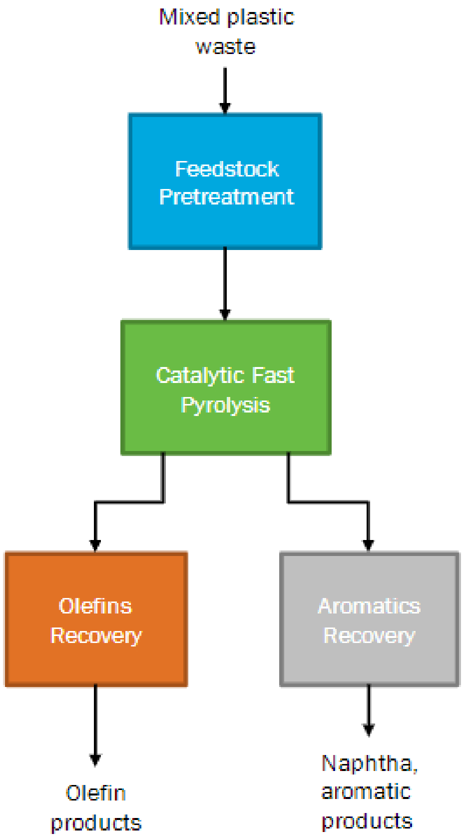
- Cost: Recycled rPET is 48% cheaper than virgin PET
- Opportunity: Cheaper feedstock and higher solvent recovery can further reduce costs
- Environmental impact: rTPA shows a 1-31% reduction across most impacts compared to vPET
- Opportunity: Increased solvent recovery and reduced pretreatment can further reduce process impacts

N.A. Rorrer *et al.*, *in preparation* 2023. * Virgin PET price higher than displayed axis range

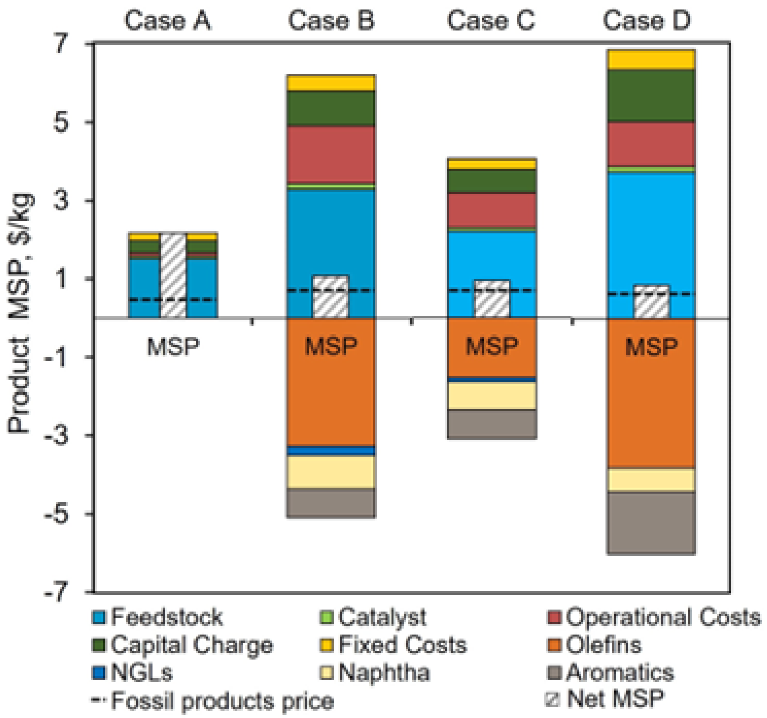
Case study III: Mixed plastic pyrolysis

Goal: Evaluate pyrolysis of mixed plastic waste as an additional benchmark for new recycling technologies

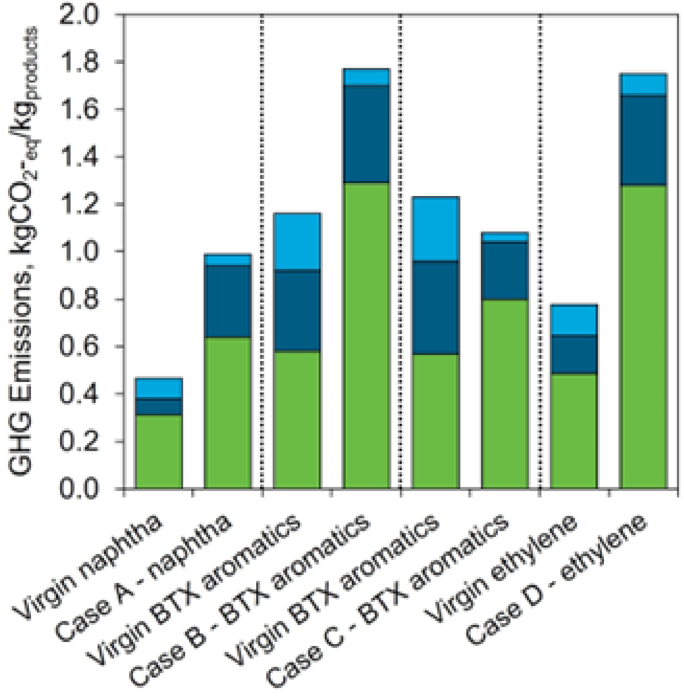
- Economics: **Naphtha, benzene-toluene-xylene (BTX), and ethylene produced by pyrolysis cost 1.5-4× virgin manufacture**
- Environmental impact: **Lower supply chain energy but higher GHG emissions and other environmental impacts**



Economic feasibility



Greenhouse gas emissions

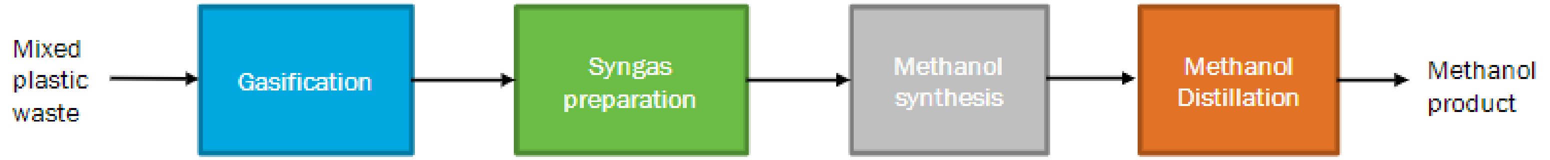


Yadav et al. *in revision*

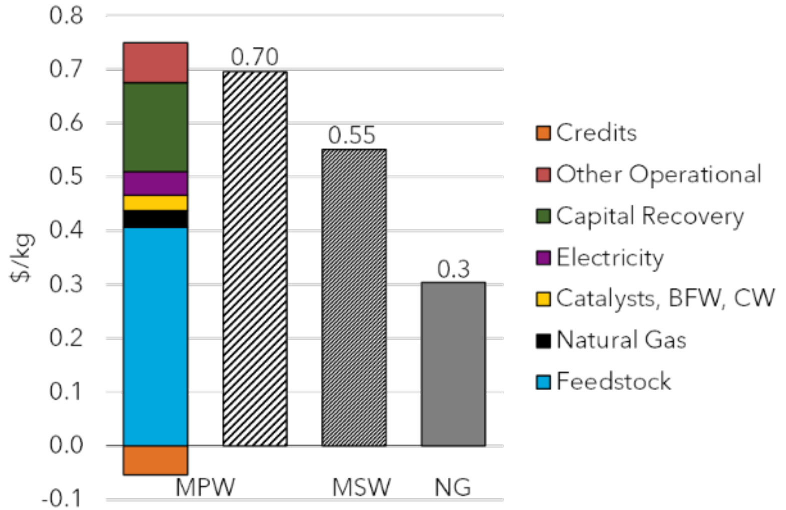
Case study IV: Mixed plastic gasification

Goal: Evaluate gasification of mixed plastic waste (MPW) and municipal solid waste (MSW) as an additional benchmark for new recycling technologies

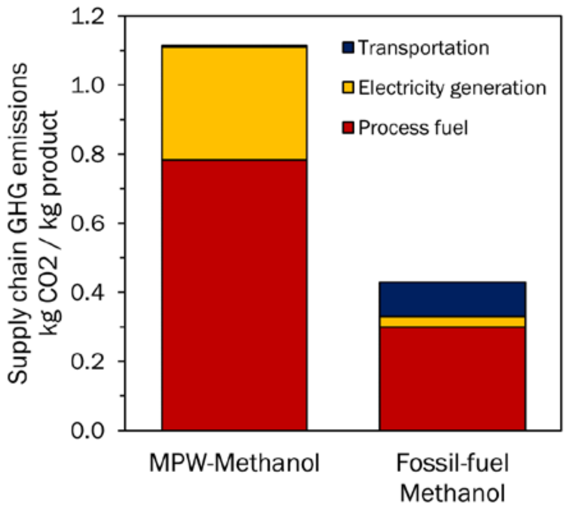
- Economics: Hydrogen and methanol produced by gasification cost 2-3× higher than virgin manufacture
- Environmental impact: Lower supply chain energy but higher GHG emissions and other environmental impacts



Economic feasibility (methanol)



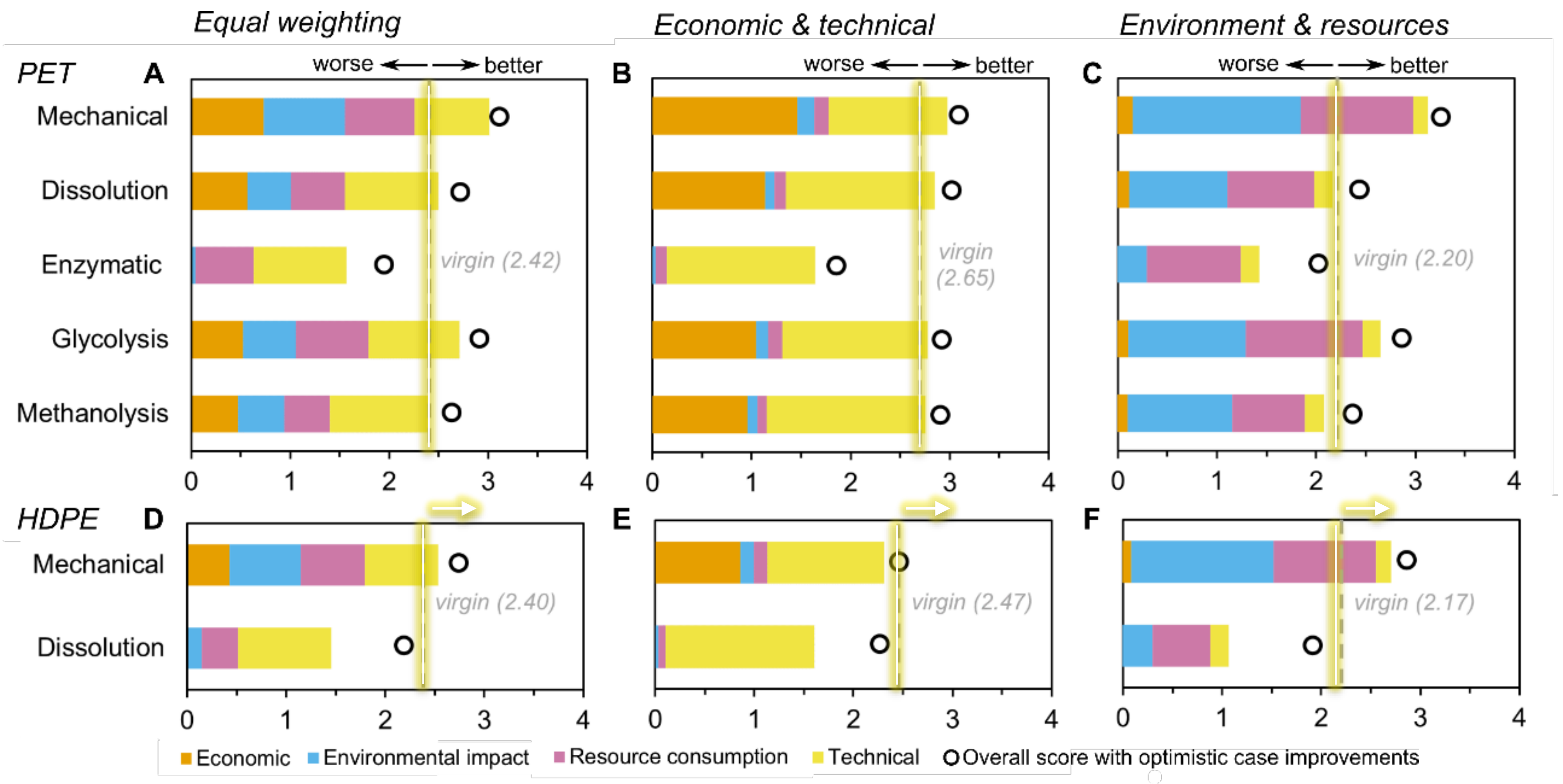
Greenhouse gas emissions



Afzal *et al. in revision*

Comparison via multi-criteria decision analysis

Goal: Compare multiple recycling technologies across multiple technical, economic, and environmental metrics.

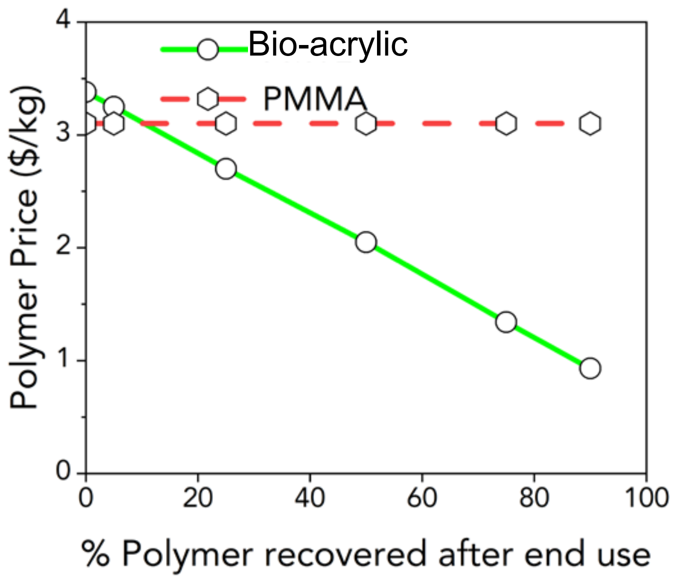


- Multi-criteria decision analysis (MCDA) – allows for the evaluation of conflicting criteria
- Some recycling technologies already offer better alternative than virgin plastic
- Technologies with low scores are not necessarily “bad” – many can improve to similar or better than virgin plastic manufacturing

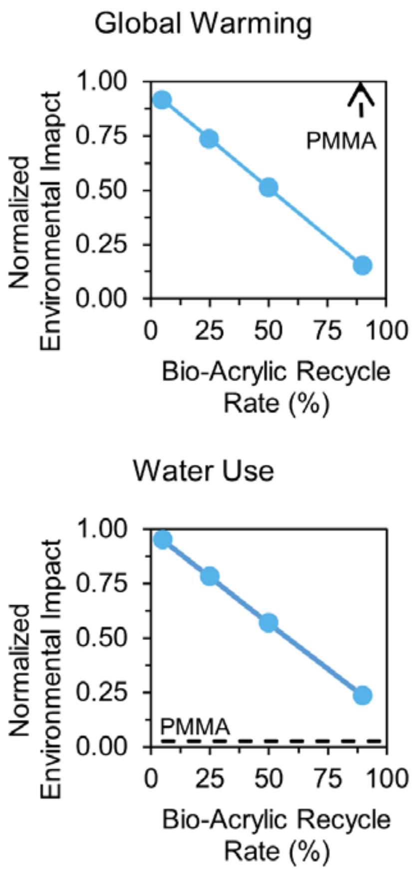
T. Uekert *et al. ACS Sustain. Chem. Eng.* 2023

Case study V: Bio-based PMMA alternative

Economic feasibility



Environmental feasibility



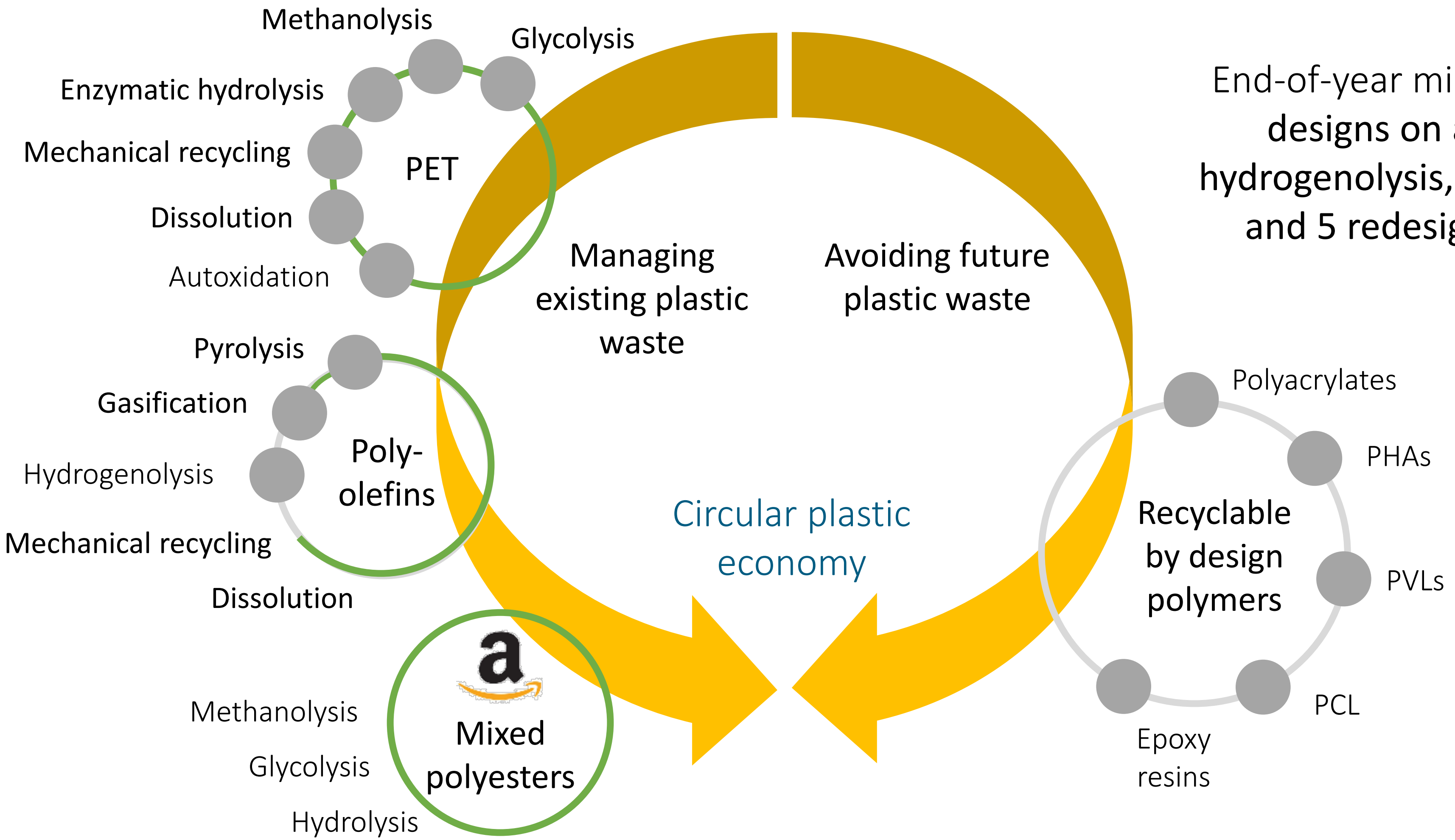
Goal: Develop an industrial-scale process model for the chemical synthesis of bio-based acrylic, a polymethyl methacrylate (PMMA) competitor.

- Cost: Bio-acrylic is cost competitive with PMMA
- Environmental impact: Bio-acrylic has similar impacts to PMMA for most categories but has 14-70× higher ozone depletion, non-carcinogenics, & water use
- Recycling: Facile thermal recycling of bio-acrylic reduces production costs and life cycle impacts
- Collaboration for optimization: Analysis work occurred in parallel to experimental work to improve the performance and scalability of the process early on

Gilsdorf *et al. in preparation*

Ongoing and upcoming analyses

End-of-year milestones: **Deliver designs on autoxidation, hydrogenolysis, PET conversions, and 5 redesigned polymers**



= stand-alone case study   = comparative analysis   = plastic family   Ongoing & upcoming analysis

Acronyms: polyhydroxyalkanoates (PHAs), polyvalerolactones (PVLs), polycaprolactone (PCL)

The impact of analysis

Inform

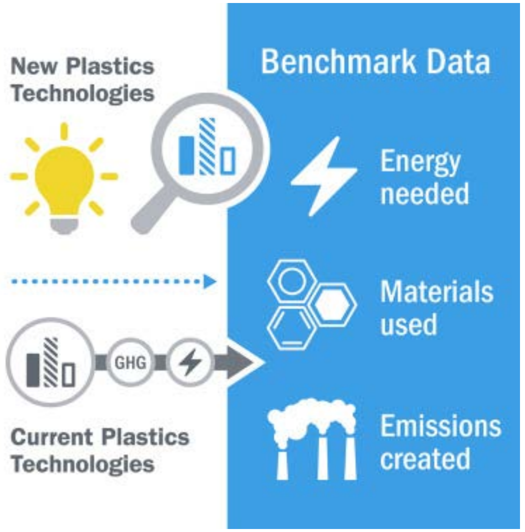
- Rigorous, transparent, consistent process modeling, TEA, and LCA
- Analysis framework serves the research community and industry
- Work in high-visibility outlets (e.g., *Joule*, *Energy Env. Sci.*, etc.)

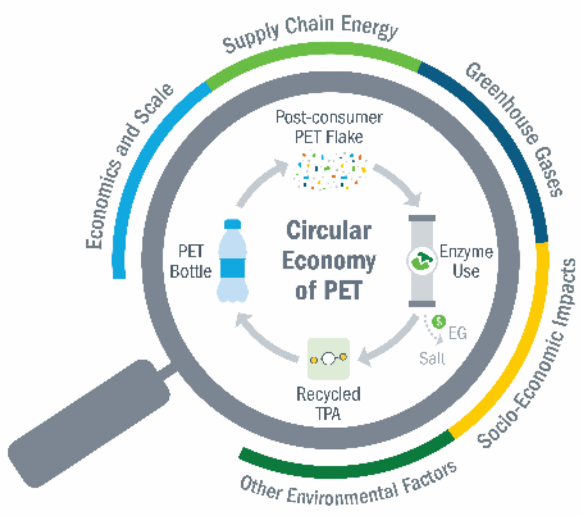
Guide

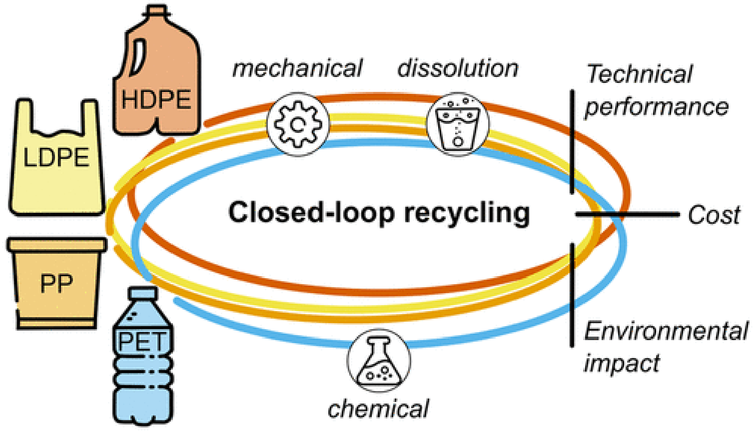
- Compare results against incumbent technologies
- Highlight research gaps and opportunities for improvement to steer resources to impact
- Used to off-board and on-board research directions

Enable

- Facilitate the deployment of technological routes towards a more circular and sustainable plastics economy
- Work with BOTTLE researchers to improve processes even 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.

Thank you!

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Publications

In preparation

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Submitted

Houqian Li, Robert D. Allen, Xianglan Bai, Gregg T. Beckham, et al., Expanding plastics recycling technologies: chemical aspects, technology status and challenges, submitted to *ACS SusChemEng.*

Publications

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Richard K. Brizendine, Erika Erickson, Stefan J. Haugen, Kelsey J. Ramirez, Joel Miscall, Davinia Salvachúa, Andrew R. Pickford, Margaret J. Sobkowicz-Kline, John E. McGeehan, Gregg T. Beckham, Effect of particle size and substrate crystallinity on enzymatic depolymerization of poly(ethylene terephthalate), in review at ACS SusChemEng.

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Presentations

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New building blocks for performance-advantaged renewable and recyclable polymers, Pacifichem (via webinar), December 2021

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Catalysis for valorization of lignin and plastics, Great Plains Catalysis Society (via webinar), June 2021

The critical role of economic and environmental analysis to guide research in lignin valorization and plastics upcycling, Keynote Invited Lecture, ACS Green Chemistry and Engineering (via webinar), June 2021

Towards Intrinsically Circular Thermoplastics and Reprocessable Thermosets, Dow Chemical Company, virtual seminar, May 2021

Recent progress in performance-advantaged bioproducts and plastics upcycling, Arizona State University (via webinar), April 2021

Recent adventures in biomass conversion and plastics upcycling, Rutgers University (via webinar), April 2021

Presentations

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