



Towards a circular economy for PET bottle resin using a system dynamics inspired material flow model

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Original research article
Think before you throw! An analysis of behavioral interventions targeting PET bottle recycling in the United States

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ADVANCED SUSTAINABLE SYSTEMS

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Comparing Parallel Plastic-to-X Pathways and Their Role in a Circular Economy for PET Bottles

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Towards a Circular Economy for PET Bottles in the US – 4P framework



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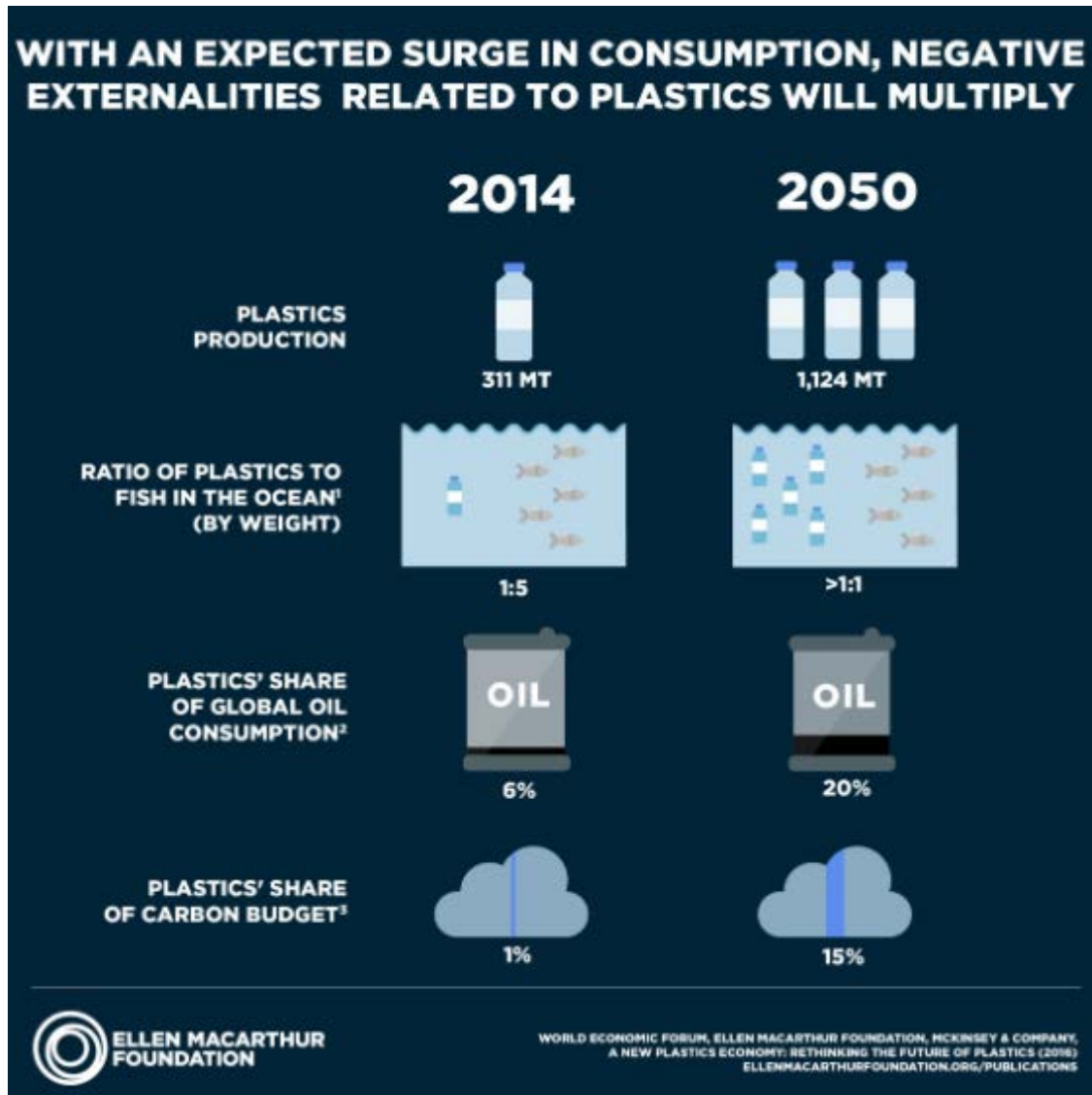


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Motivation – the “decarb” angle



5% of plastic waste in U.S. is recycled¹

Data gaps:

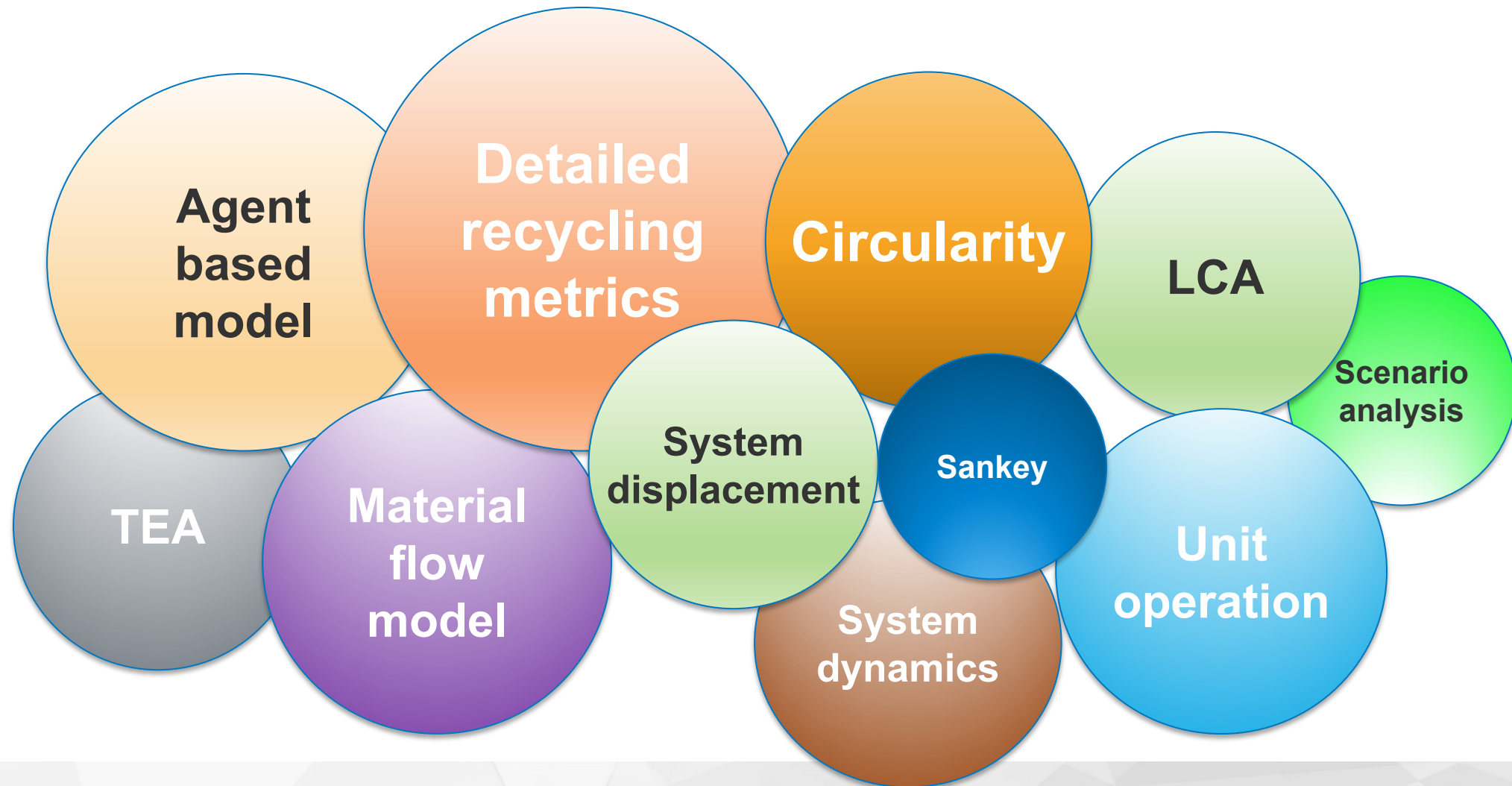
- Technical capabilities, cost, environmental impact of recycling strategies
- Plastic waste collection – current status and how to improve
- What about other upcycling, downcycling, or even reuse strategies? How can we compare and pick the best?

Objectives

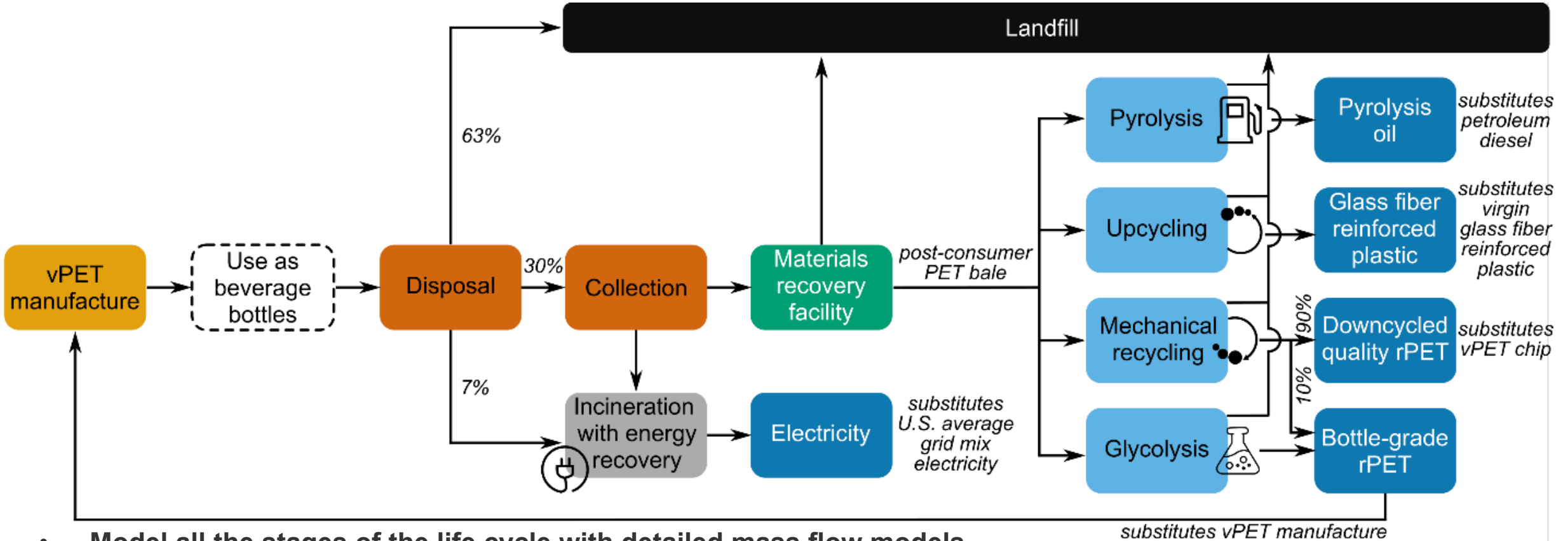
Develop a framework capable of quantitatively comparing the plastic end-of-life strategies that generate different products.

- Tracking the flow of plastics in the economy within single and multiple life cycles.
- Implementing metrics for measuring circularity for complex systems.
- Process-based life cycle assessment (LCA) to compare circular solutions' environmental impacts
- Techno-economic analysis (TEA) of end-of-life pathways.

Plastic Parallel Pathways Platform – a systems analysis tool for plastics end-of-life management



Plastic Parallel Pathways Platform– 4P Model



- Model all the stages of the life cycle with detailed mass flow models
- Model of the constraints mathematically
- Model substitution of virgin with recycled resin, electricity from incineration, diesel fuel and reinforced polymer resin
- Model novel recycling pathways
- Improve regional resolution
- Calculate circularity and LCA indicators.

Plastic circularity index

Linear Flow Index

The Linear Flow Index (LFI) measures the proportion of material flowing in a linear fashion, sourced from virgin materials and ending up as unrecoverable waste.

$$\text{LFI} = \frac{\text{Linear flow}}{\text{Total Flow}}$$

Utility Factor

A utility factor (X) is incorporated, which considers both the product lifetime (L) and product utility, or the extent to which a product is used to its full capacity (U)

$$X = \left(\frac{L}{L_{av}} \right) \left(\frac{U}{U_{av}} \right)$$

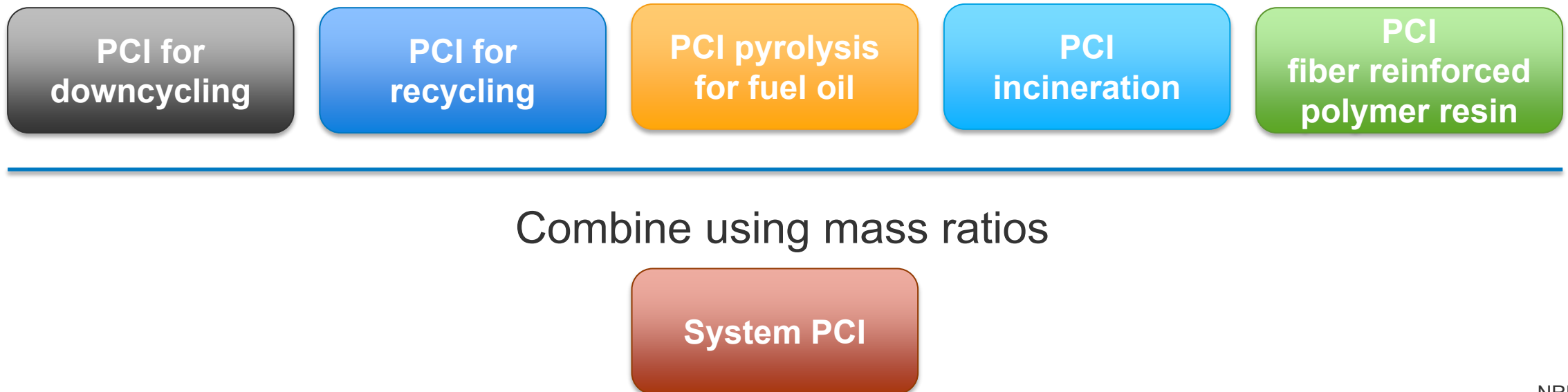
Where L_{av} is the industry average product lifetime and U_{av} is the industry average product utility.

Plastic circularity index

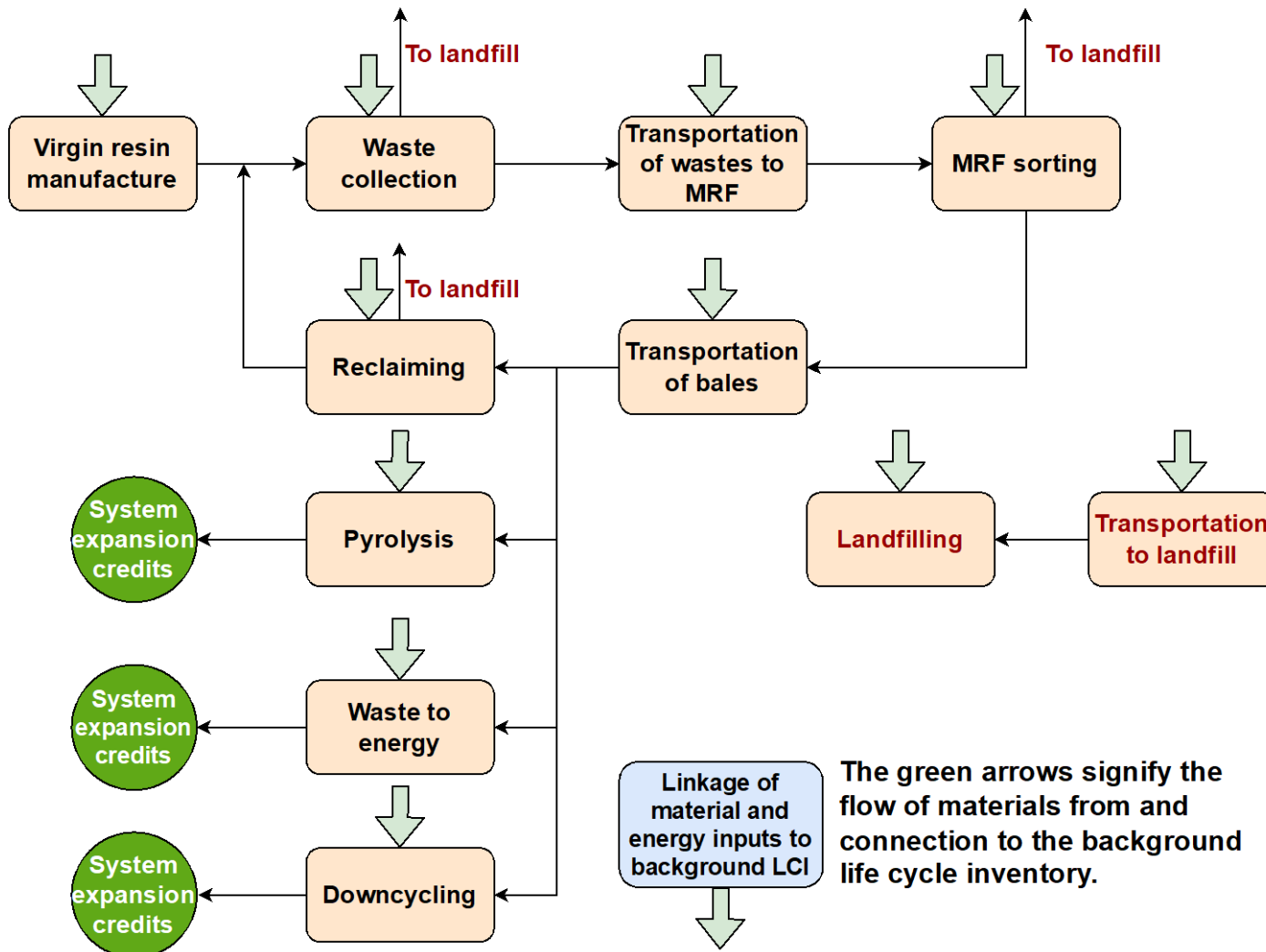
Plastic circularity index is defined by considering the linear flow index of the product and a factor $F(X)$, built as a function of utility X . The product's utility is captured using the X .

$$PCI = 1 - \left(LFI \times \left(\frac{0.9}{X} \right) \right)$$

PCI is calculated for the entire system for every time step in the model.



Life cycle assessment



- PyLCIA* – Python based Rapid LCA (Prospective LCA performing 1000s of calculations with evolving inventory – background as well as foreground changes with time)
- Foreground system – Activities in the material flow model
- Background system – US life cycle inventory¹
- Electricity provider – ReEDS² dynamic grid mix utilized for foreground system electricity consumption
- TRACI 2.1³ LCIA methodology adopted

* Ghosh, Tapajyoti, et al. "Towards a circular economy for PET bottle resin using a system dynamics inspired material flow model." *Journal of Cleaner Production* 383 (2023): 135208.

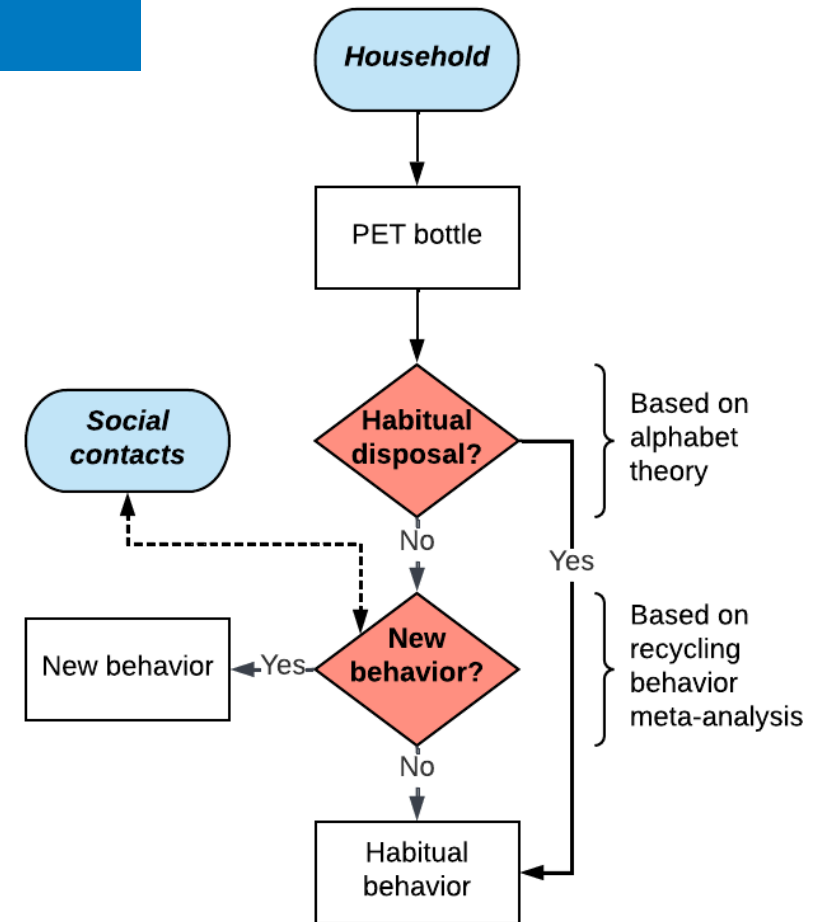
1. "U.S. Life Cycle Inventory Database." (2012). National Renewable Energy Laboratory, 2012. Accessed November 19, 2012: <https://www.lcacommons.gov/nrel/search>

2. <https://www.nrel.gov/analysis/reeds/> 3. <https://www.epa.gov/chemical-research/tool-reduction-and-assessment-chemicals-and-other-environmental-impacts-traci>

Agent based model for collection rate

ABM models human behaviors

- **Objective:** model household recycling behaviors under different intervention scenarios (e.g., increased access to curbside recycling programs or cart-tagging campaigns)
- **Scope:** trash, recycling, and "wish-cycling" of PET with up to Census Block Group geographic resolution
- **Methodology:** Model the habitual nature of disposal behaviors and agents have a chance to "ponder" their action based on factors from a meta-analysis on recycling behavior



**Decision tree
representing agents'
behavioral rules**

Parameters and Scenarios

Landfill diversion

Waste incineration diversion

Mechanical recycling diversion

Chemical recycling diversion

Chemical upcycling diversion

Pyrolysis diversion

Polyester diversion

Recovery mechanical recycling

Recovery chemical recycling

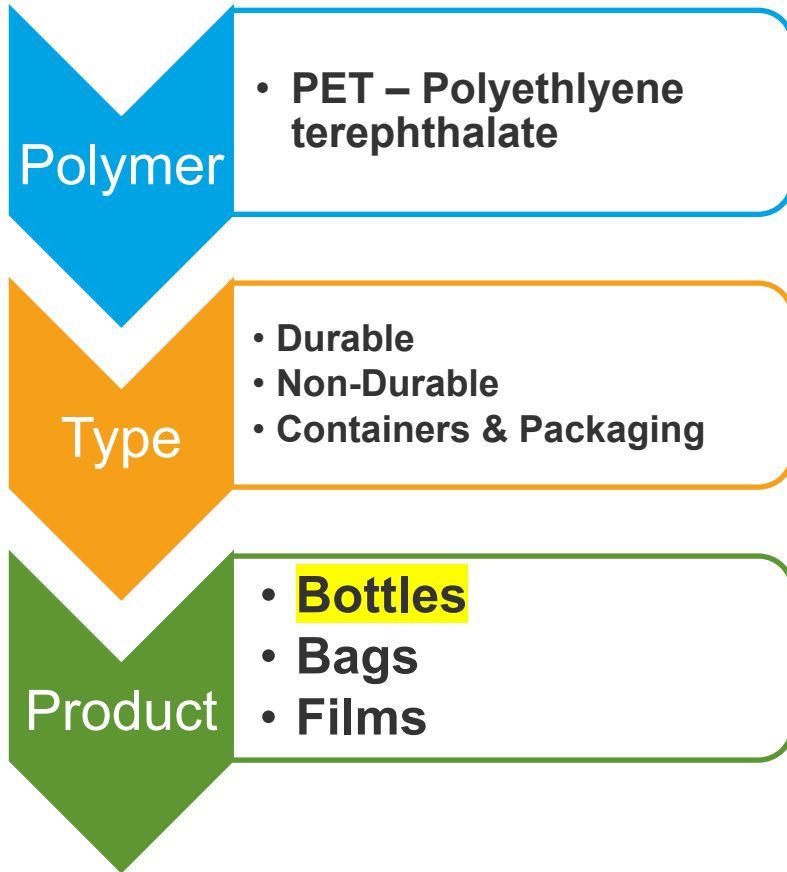
Material recovery facility equipment efficiency

Collection rate variables / ABM

Selectivity of recycled PET

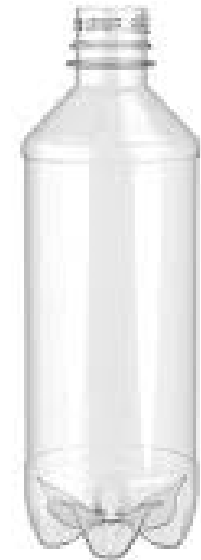
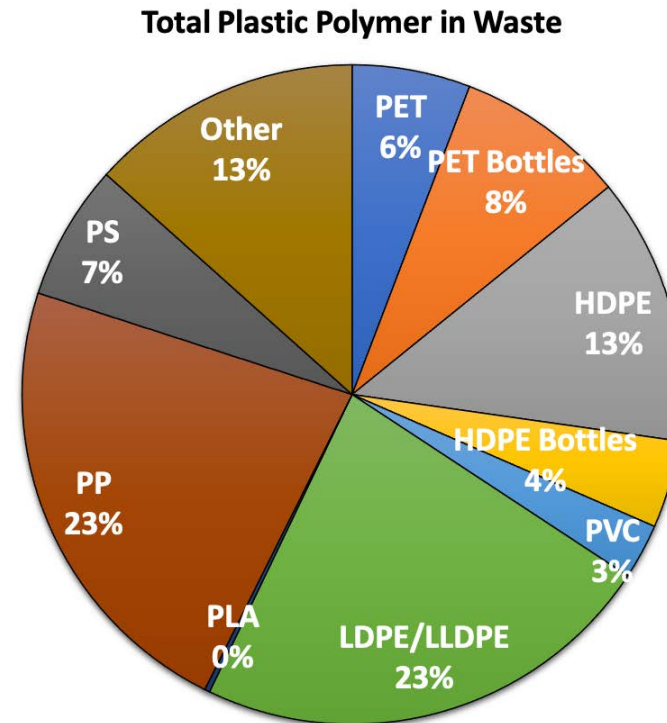
Scenarios can be created by adjusting the parameters using the data driven framework. Scenario creation is easy and once built can be saved for future use. Scenarios can be created both by changing parameters per scenario as well as with time (yearly) for a single scenario.

Case study– PET bottles

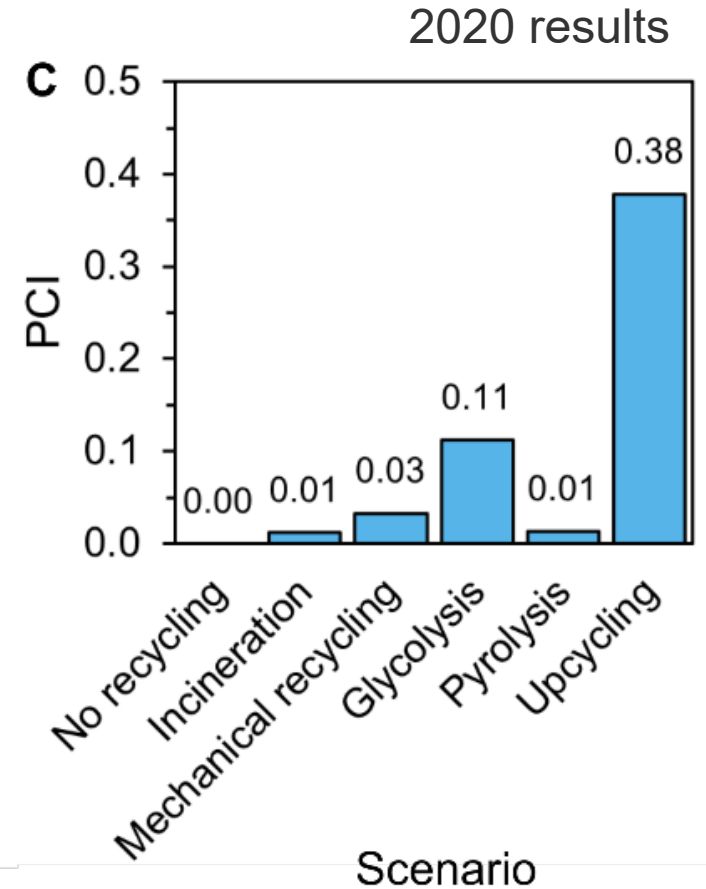
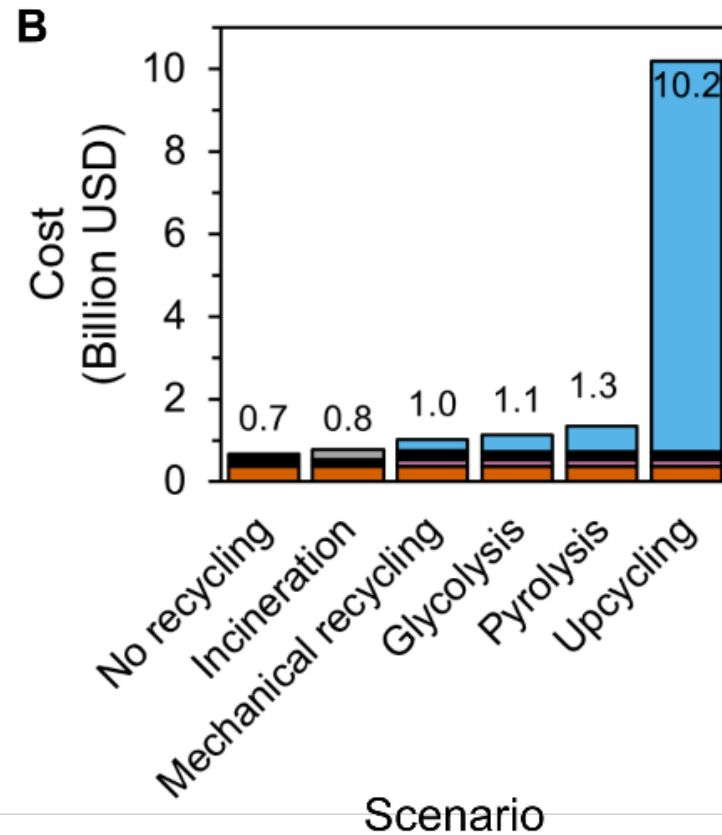
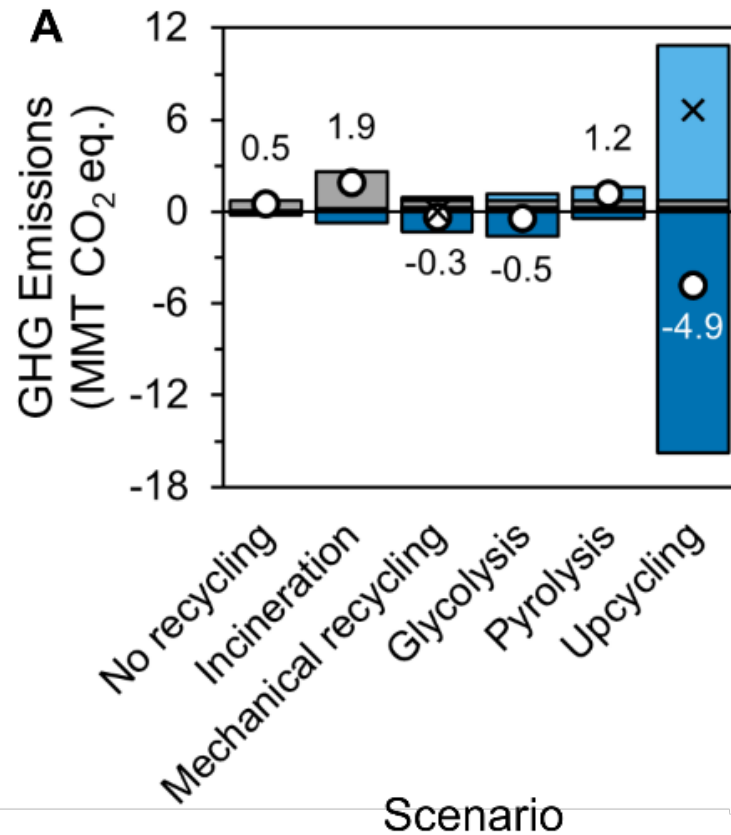


The framework is capable of handling only one resin and one product at a time.

End of life processing is dependent on resin as well as the product produced from it.



Comparison of scenarios

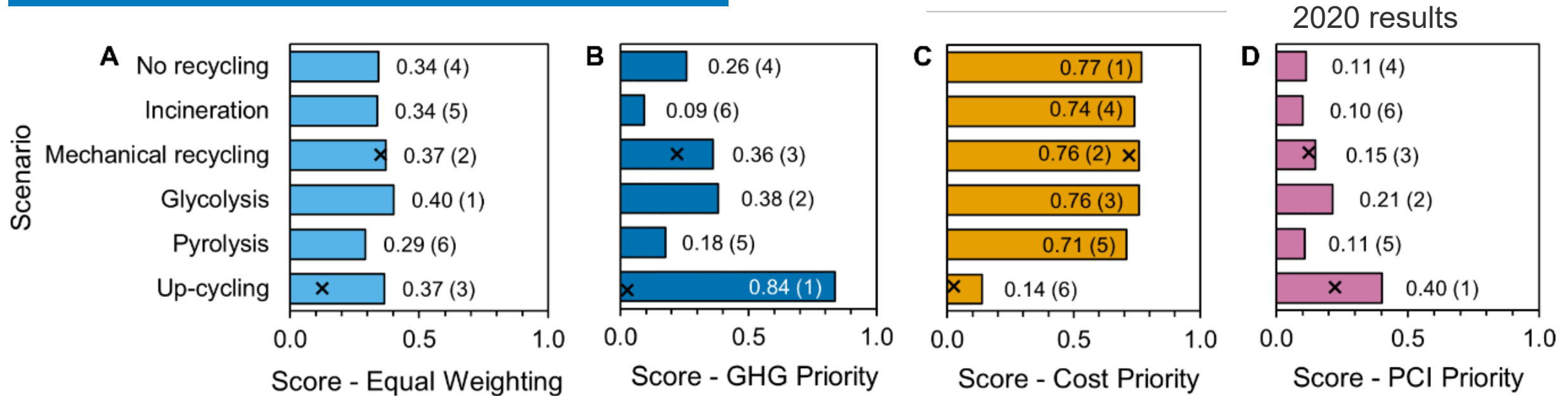


Collection
 MRF
 Transportation
 Landfill
 Incineration
 Recycling or upcycling

Displaced product
 Net
 Net with market-constrained displaced product credits

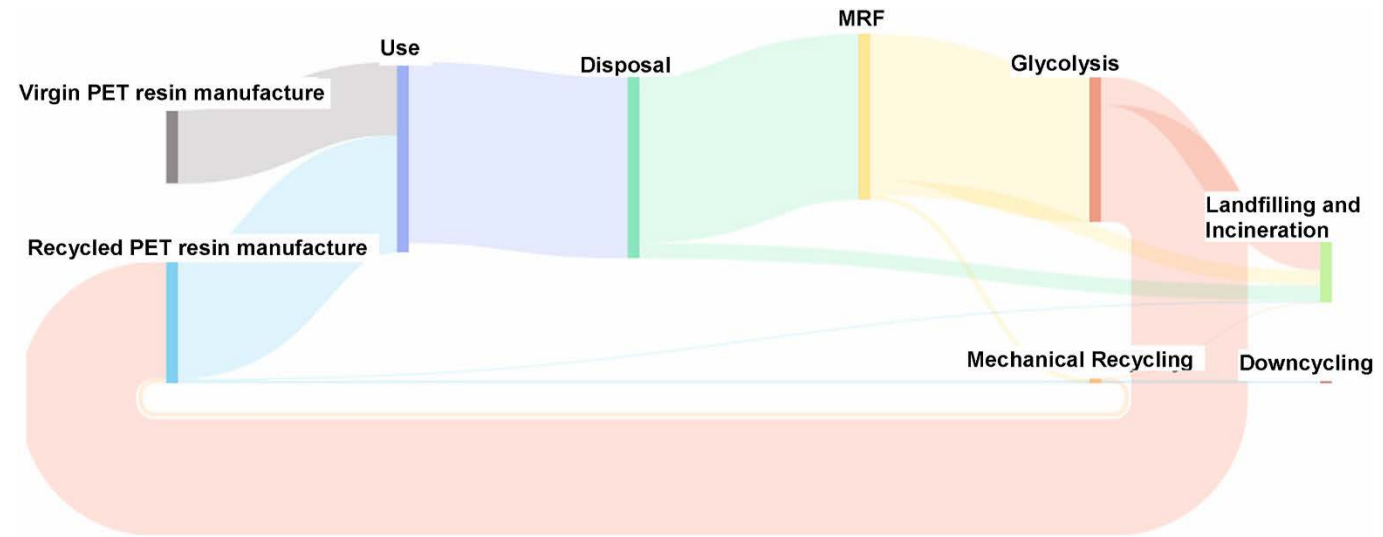
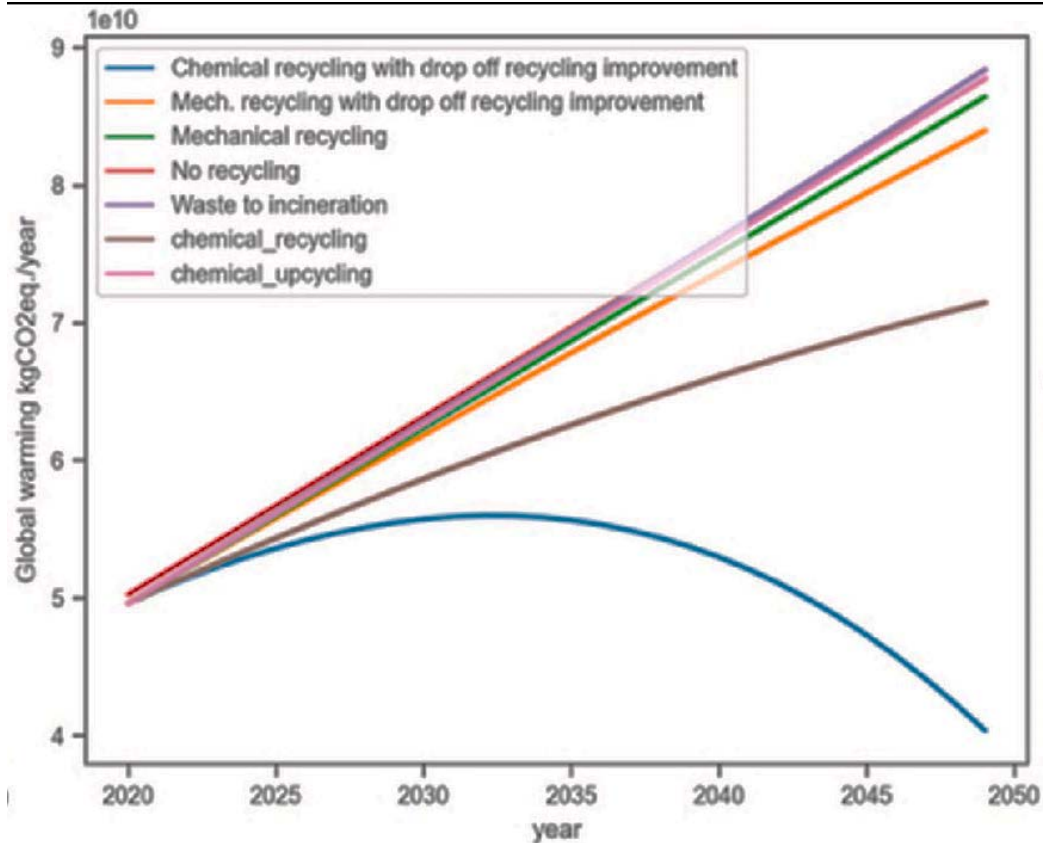
Comparison of the (A) GHG emissions, (B) cost, and (C) PCI if all PET bottles collected for recycling in the U.S in 2020 were used to produce lower-quality PET resin by mechanical recycling, food-grade PET resin by glycolysis, electricity from incineration, fuel oil from pyrolysis, or fiber-reinforced resin by upcycling.

Multi criteria decision analysis



- Providing weights to the values of GHG impacts, Cost and Plastic Circular Index and combining them to provide final scores for decision making.
- The EoL pathways with the best balance of all metrics – glycolysis and mechanical recycling – therefore emerge as the most favorable.
- The close scores across most scenarios could indicate that there is no “best” technology under the assessed criteria.
- Designing the end-of-life PET recycling industry will require a combination of pathways chosen according to variety of factors – infrastructure availability, regional requirement, cost viability and others.

Simulation from 2020 to 2050 across different mitigation scenarios (accounts for total PET usage over time)



The 4P framework analyzes different pathways of recycling technology deployment, mitigation scenarios and compares overall improvement in environmental impact, circularity and cost with time.

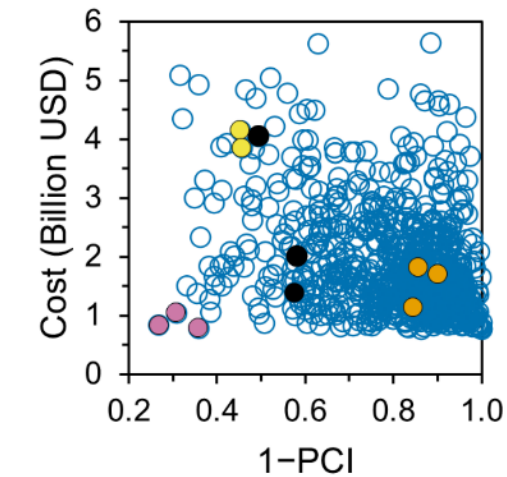
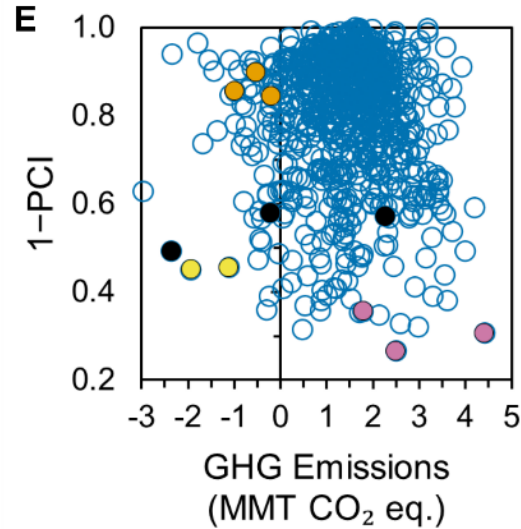
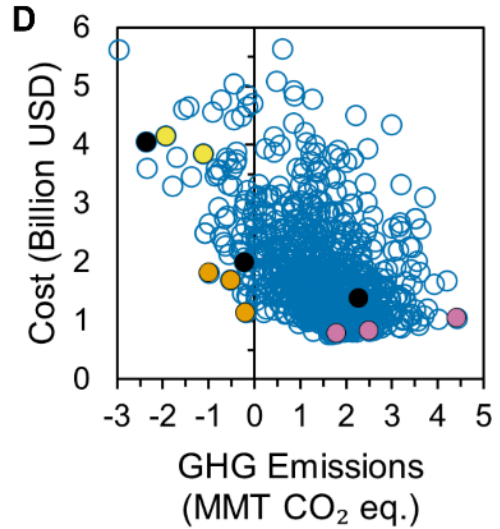
Even with PET bottle usage increase over time, its possible to reduce absolute GHG footprint of the PET bottle life cycle with deployment of chemical recycling and improvement of waste collection by improving drop off recycling availability to consumers via displacement of virgin PET resin.

Uncertainty quantification

- 4P can also design systems while accounting for uncertainty in the system parameters.
- Upper and lower bounds are provided for the parameters.
- A triangular distribution is assumed for each of these parameters as there is insufficient data to predict a more accurate probability distribution function.
- For each run of 4P, a sample is randomly drawn from the distribution for the parameters as well as from the uniform distribution of design variables.
- Uncertainties of system parameters only.

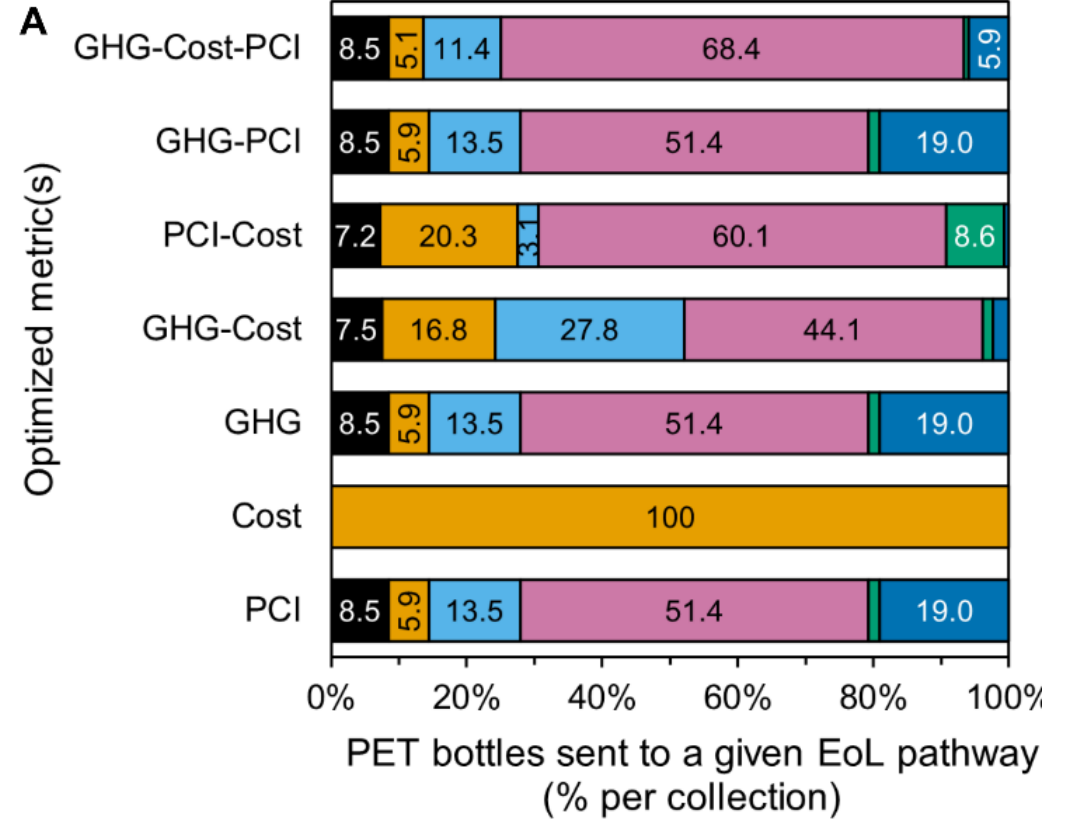
Brute force optimization for exploration of pathways

2020 results



Exploring the solution space by imposing uncertainty on system parameters and varying the design variables.

- Low GHG, Low Cost, High PCI
- Low GHG, Low Cost
- Low GHG, High PCI
- Low Cost, High PCI



Designing the US plastics recycling system with spatial resolution



4P

Material Flow model, Life cycle assessment, TEA, Circularity, System dynamics



RELOG

Supply chain optimization, Capacity expansion, Reverse logistics, Reverse planning

- Capacity expansion model.
- Spatial resolution limited by data availability.
- Location and expansion of new MRFs, reclaimers, product manufacturers.
- Integration with existing facilities.
- Assessment of end-of-life pathways.
- Design solutions for recycling targets.
- Other plastic polymers - HDPE

Conclusions

- Development of a plastic material flow model framework that can track the flow of individual plastic resin through different stages of end-of-life processing.
- Circularity, environmental impacts and cost are calculated in a **prospective manner**.
- End-of-life products are combined to calculate **system circular index**.
- While upcycling stands out as the better pathway via multi criteria indicator analysis, considering market constraints on product demand shows glycolysis and mechanical recycling as more attractive choices.
- With **chemical recycling and improvement of waste collection**, its possible to reduce absolute GHG emissions with displacement of virgin PET manufacture.
- The 4P framework can design end of life recycling pathways for variety of metrics and combination of indicators.



Thank you

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Other end-of-life pathways

Chemical
recycling
via
glycolysis

Pyrolysis
to produce
plastic
pyrolysis oil

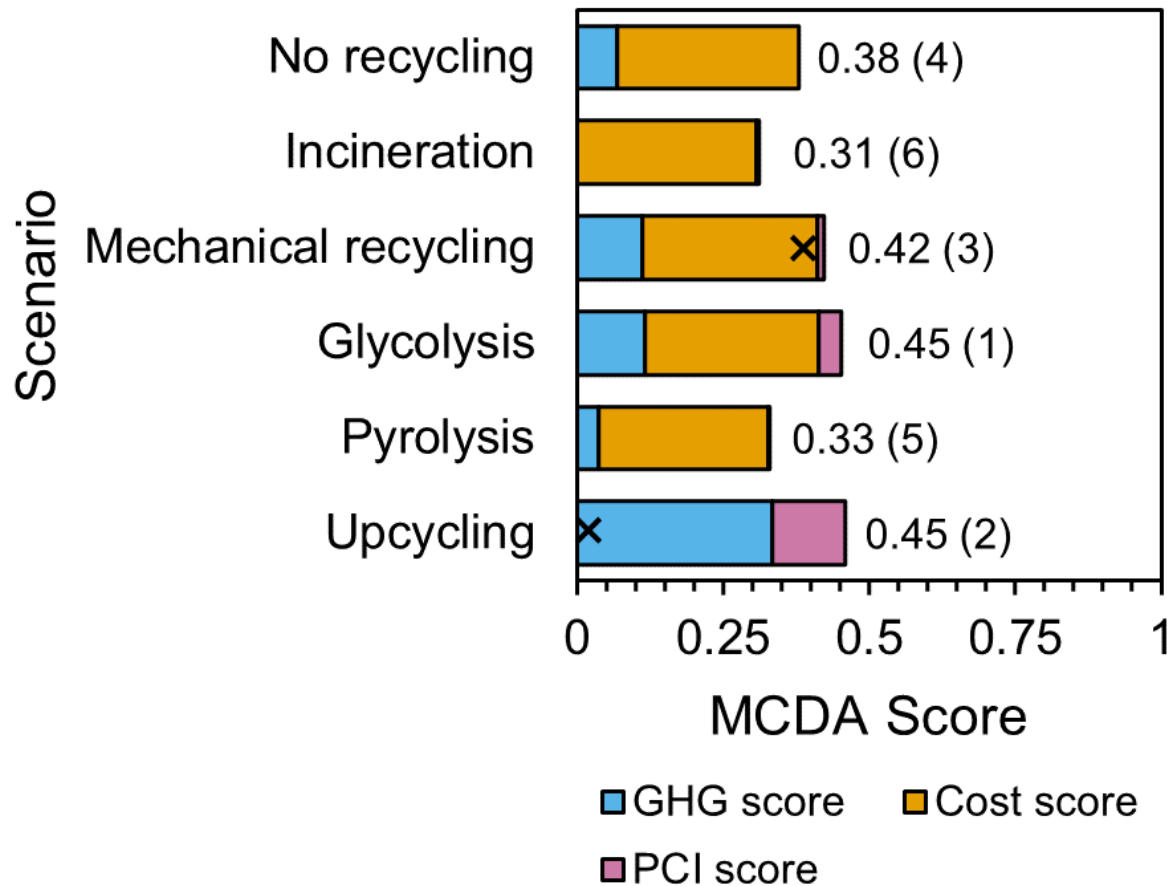
Upcycling to
produce
resin for
reinforced
polymer

Incineration
to produce
electricity

Model:

Linear models with *parameters* for conversion, recovery and loss

Multi criteria decision analysis



The black x's indicate MCDA scores for mechanical recycling and upcycling when GHG emission displacement credits are capped at the market demand for PET chip and GFRP, respectively

- The EoL pathways with the best balance of all metrics – glycolysis and mechanical recycling – therefore emerge as the most favorable.
- The close scores across most scenarios could indicate that there is no “best” technology under the assessed criteria.
- Furthermore, the uncertainty of such MCDA estimates is high.