Reinventing the Chemicals and Materials Industry for a Net-Zero, Nature-Positive World

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Energy Systems Initiative, Center for Advanced Process Decision-making Carnegie-Mellon University October 12, 2022

Role of the Chemicals and Materials Industry

Top 10 Chemical Engineering InventionsChemical Engineering Inventions1. Drinking or potable water2. Petrol or gasoline (and other fuels including diesel)3. Antibiotics4. Electricity generation (from fossil fuels)5. Vaccines6. Plastics7. Fartilizer

- 7. Fertilizer
- 8. Sanitation
- 9. Electricity generation (from non-fossil fuels)
- 10. Dosed medication (such as tablets, pills, capsules)

Chemical Industry Contributes

- \$5.7 Trillion to global GDP
- Supports 120 million jobs
- Direct contribution of \$1.1 trillion and 15 million jobs

https://www.icca-chem.org/economicanalysis/

Inst. Chem. Eng., 2014

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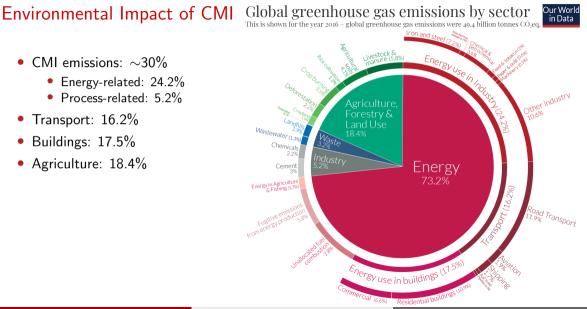
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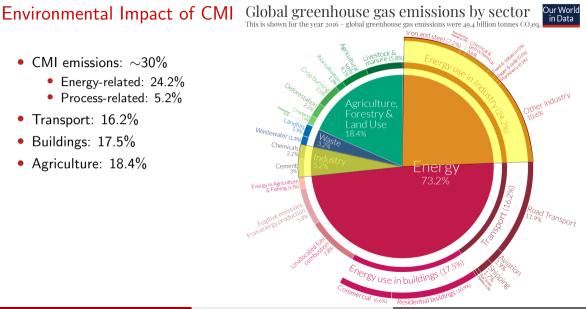
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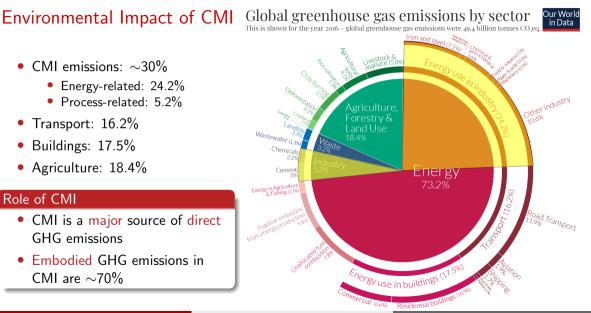
In summary,

- CMI is essential for human well-being
- However, it also results in a large negative impact

Inst. Chem. Eng., 2014





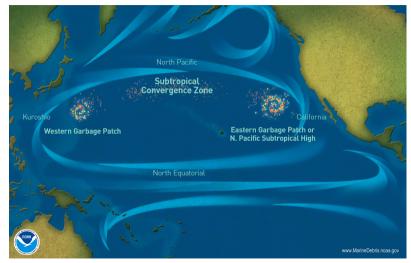


Environmental Impact of CMI: Plastics

- Plastic islands in the ocean
- Plastic litter in Hawaii



(US Fish and Wildlife Service)



http://marinedebris.noaa.gov

Net-Zero, Nature-Positive, Socially Just

Interconnected crises facing the world require efforts toward,

- Net-Zero for addressing emissions and resource use
 - Greenhouse gas emissions and climate change

- Nature-Positive for addressing ecological degradation
 - Loss of biodiversity, ecosystem goods and services

- Socially Just for addressing social inequities
 - Shortfalls in human well-being

Net-Zero: Pledges and Problems

• Corporations have pledged net-zero greenhouse gas emissions

Net-Zero: Pledges and Problems

 Corporations have pledged net-zero greenhouse gas emissions

obeNEWS	VIDEO	LIVE	SHOWS	CORONAVIRUS	JAN. 6 RIOT	OLYMPICS	New York Times
	e	missi	ons by	npanies p 2040 as j r mounts			
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	-			in the wake of a di	re warning from a	UN climate panel	Exxon Sets

In 28 Years By CLIFFORD KRAUSS HOUSTON – Exxon Mobil, under increasing pressure from investors to address climate change, announced on Tuesday that it had the "ambition" to reach zero net greenhouse gas emissions from is operations by 2050. The oil company, the largest in the United States, still remains be-

Updated 4:25 PM FT, Mon February 7, 2022

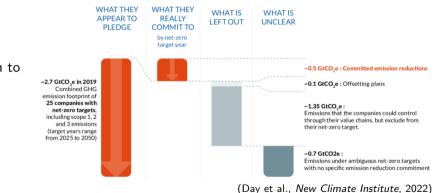
Net-Zero: Pledges and Problems

- Corporations have pledged net-zero greenhouse gas emissions
- However, they seem to be falling short

Over 200 companies pledge net-zero emissions by 2040 as pressure on private sector mounts The announcement comes in the wake of a dire warning from a UN climate panel. Image: State of the sector mounts Image: Stat	Sets Goa
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💌 DOW 34,738.08 -503.53 -1.43%	
TS&P 500 4.418.84 -65.44 -1.90% From jobs to GDP, these key indicators provide a comprehensive, Cisco makes \$20 billion-plus takeover offer for Splunk	KRAUSS Mobil, und
* NASDAO 13,781.15 -394.49 -2,78% up-to-data picture of the US Economy. Super Bowl ticket prices have dropped but they'll still cost you thousands	From investite change, a
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Some of the world's hiddest companies are failing on their ow	
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Net-Zero: Pledges and Problems

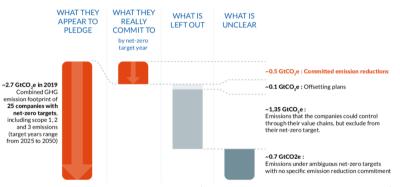
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Integrity of Corporate Net-Zero Pledges

Net-Zero: Pledges and Problems

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- However, they seem to be falling short
- Progress toward nature-positive decisions is even slower



Integrity of Corporate Net-Zero Pledges

(Day et al., New Climate Institute, 2022)

Research Motivation and Goal

For CMI to become net-zero and nature-positive while remaining economically viable,

- Small adjustments of the current system will not be enough
- CMI must be reinvented to a circular enterprise
- Engineering paradigm must shift to accounting for nature and respecting its limits

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Overall Goal of Research

Develop systematic methods and tools to transform engineering so that its contributions are,

- ecologically viable
- economically feasible
- socially desirable

for current and future generations

Eco-Mimicry

- Learn from and emulate nature
- Enable a net-zero, circular economy for materials and products

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- Include nature in engineering and LCA
- Encourage nature-positive decisions that protect and restore ecosystems

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Sustainability Transitions

- Guide transition to sustainability
- Develop roadmap of path toward meeting sustainability goals

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Safe and Just Process Engineering

- Respect nature's capacity and social equity
- Formulate novel metrics and designs

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Multiscale Sustainable Engineering

- Provide theoretical foundation
- Framework to integrate models from molecular to planetary scales

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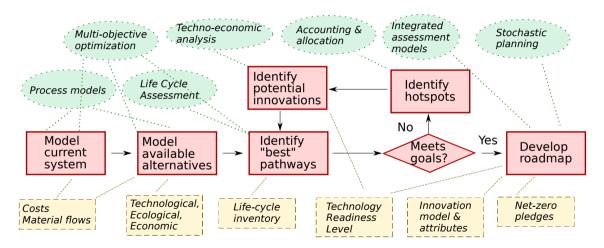
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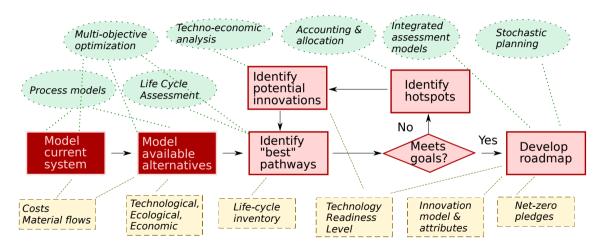
Sustainability Education

- Train students and professionals
- Develop teaching material, courses, books

Framework for Progress Toward Net-Zero CMI



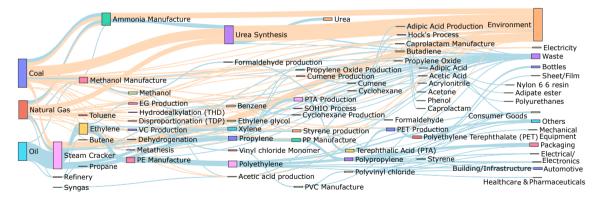
Framework for Progress Toward Net-Zero CMI: Model Current System



Toward Net-Zero CMI

Model Current System: Global Chemicals and Materials Industry

- Direct carbon flow in the global chemical industry
- Carbon efficiency: 42%

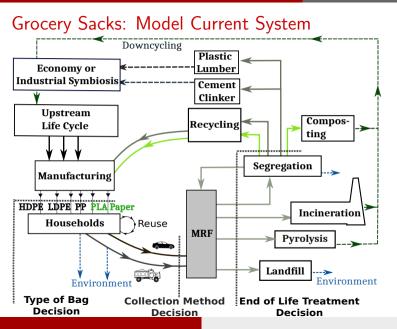


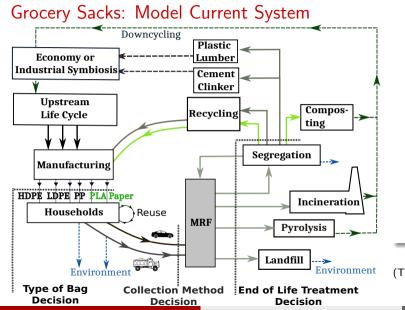
(Sen, Stephanopoulos, Bakshi, AIChE meeting, 2021)

Net-Zero GHG Emissions: Which Grocery Sack?



Plastic (LDPE, HDPE, PP, PLA), paper, cotton, something else?

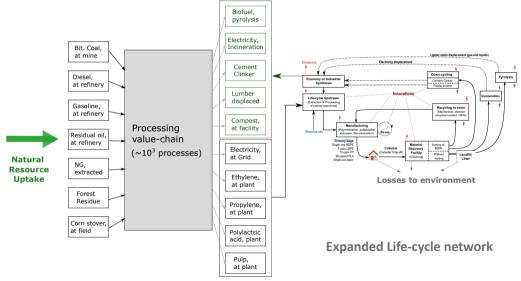




- Each step has many alternatives
- Each combination of alternatives has different,
 - Circularity
 - Life cycle impact
 - Cost
- Which pathway is best?
- How do we innovate for circularity?

(Thakker and Bakshi, ACS SCE, 2021)

Expanded Superstructure for SCE Design of Grocery Bags



Framework for SCE Design: Optimization Problem

$$\min_{s,a_{im},a_{nj}} z := Z(\cdot)$$

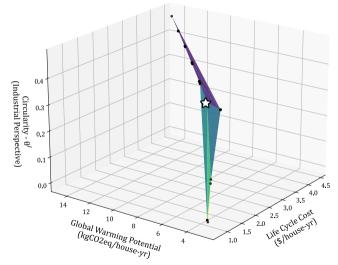
s.t. $As = f$
 $g = Bs$
 $Hs \ge u$
 $\mathcal{F}(\cdot) = 0$
 $f_k \in \mathbb{R} \ \forall \ k \in c$
 $f_k = const \ \forall \ k \notin c$
 $s \ge 0$

Single or multiple objectives

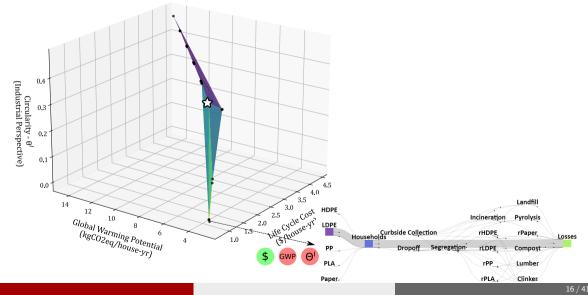
Life cycle network Life cycle impact Consumer requirements Governing Equations

(Thakker and Bakshi, J. Cleaner Prod., 2021)

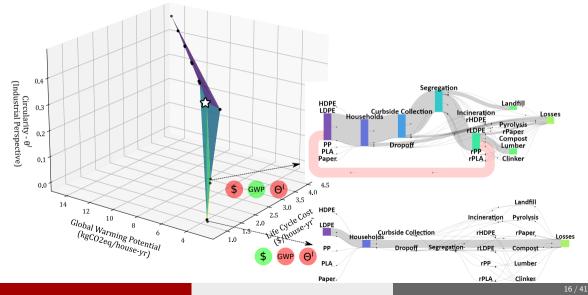
Framework for SCE Design: Application to Grocery Sacks

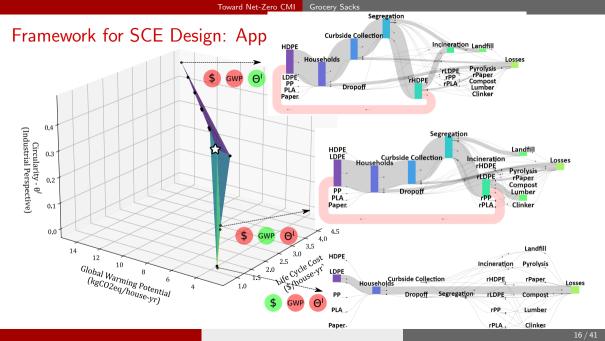


Framework for SCE Design: Application to Grocery Sacks

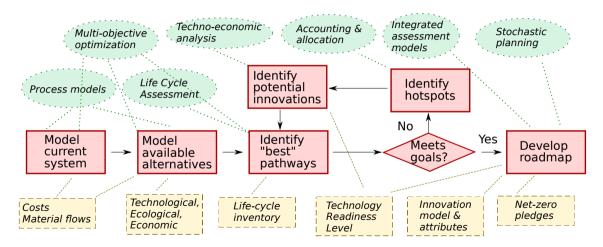


Framework for SCE Design: Application to Grocery Sacks

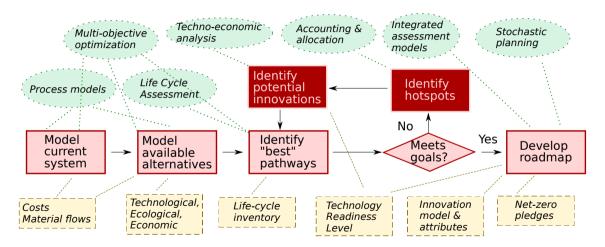




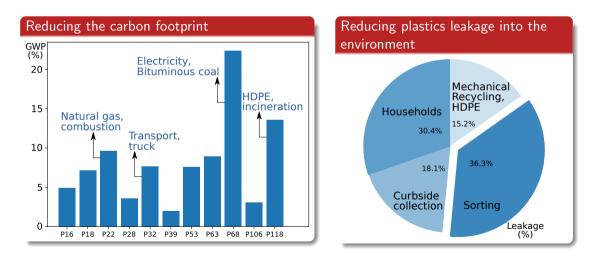
Framework for Progress Toward Net-Zero CMI



Framework for Progress Toward Net-Zero CMI: Hotspots and Innovations

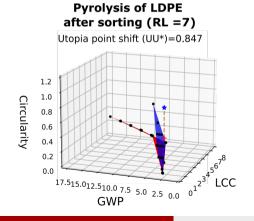


Identifying Opportunities for Improvement

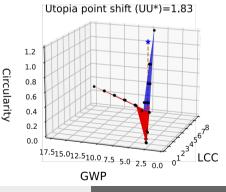


Screening and Ranking of Innovations

- Identified 100+ alternatives in grocery bags' value chain (Hafsa et al., J. Cleaner Prod., 2022)
- Determine potential effect of new technologies by comparing Pareto surfaces
- Consider technology readiness levels



Chemical recycling of PLA to LA using ionic liquids (RL =2)

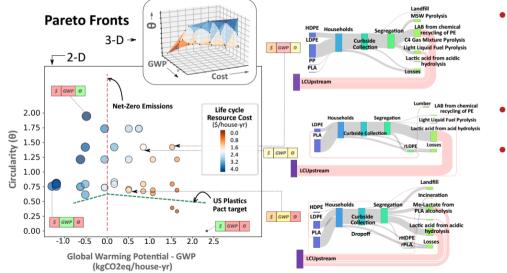


Innovations Relevant to Grocery Sacks

Rank	Innovation name	Readiness level	UU*	Ranking criterion
1	Catalytic pyrolysis of segregated LDPE	7	0.85	0.621
2	Alkaline hydrolysis of PLA to LA using ionic liquids	2	1.83	0.611
3	Linear alkyl benzenes from sorted PE	2	1.83	0.610
4	Bio-polyethylene from sugarcane based	7	0.8	0.603
	bio-ethanol harvested in Brazil			
5	Source segregation by consumers	7	0.41	0.500
6	Catalytic pyrolysis of segregated PP	5	0.7	0.469
7	Alcoholysis of PLA	5	0.59	0.439
8	Catalytic pyrolysis of segregated HDPE	6	0.38	0.436
9	Chemical recycling of PLA to polymer using mononitrile clay, Sn/Toluene	3	0.18	0.216

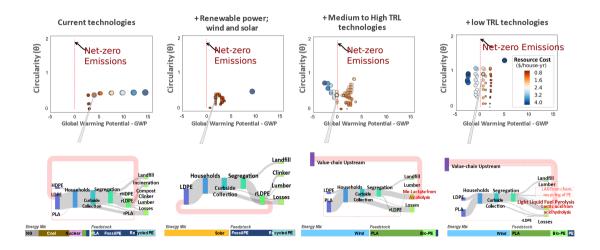
(Thakker and Bakshi, ACS SCE, 2022)

Future Grocery Sacks: Sustainable, Circular, Net-Zero

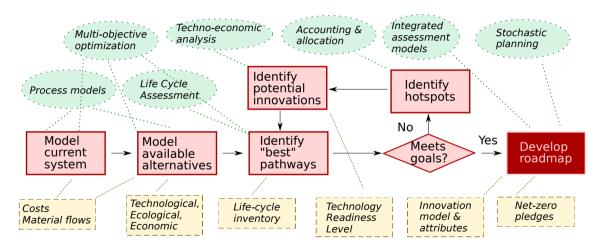


- Grocery bags with net-zero CO₂ and high circularity are possible
- Likely to cost more
 - Need
 research and
 development

Evolution of Grocery Sacks with Advances in Technology



Framework for Progress Toward Net-Zero CMI: Develop Roadmap



Develop Innovation Roadmap: Planning Optimization framework

 $\min_{x,y,t} z := \text{ Operating Cost } + R\&D \text{ Cost } =$

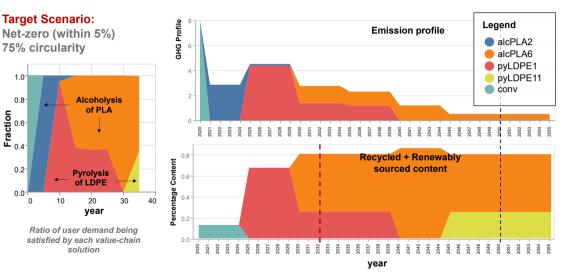
$$\sum_{tt} \left| \sum_{k \in \text{ Pareto-set}} \text{ Cost }_{\text{Resource use from } k} + \sum_{i \in \text{inn}} \text{ Cost }_{\text{perRL of } i} \left\{ RL_{\text{max}} - \mathbb{E}\left[RL_{i} \right] \right\} \right|$$

s.t.
$$f(x, y, t, tt) \ge 0,$$

 $RL_i = g_i(t, tt, \cdot) \ge 0$
 $A(t) = h_i (A_0, \text{RCP}_{2.6}, t)$
 $CO_2 (x, y, t^{2050}) \le 0$
Circularity $(x, y, t^{2030}) \ge 0.5$
 $\sum_{i, t_i} k (x_i t_i, tt) \le B$
 $y \in \mathbb{Z}, x = \mathbb{R} \in \{0, 1\}$
 $t \in \mathbb{R}, tt \in \mathbb{Z}$

Multi-Period Planning Constraints Continuous-time Markov Chains Integrated Assessment Models Climate Change Target US Plastics Pact Target Accrued Emission constraints

Innovation Roadmap: Grocery Sacks



Net-Zero, Nature-Positive, Socially Just

Interconnected crises facing the world require efforts toward,

- Net-Zero for addressing emissions and resource use
 - Greenhouse gas emissions and climate change

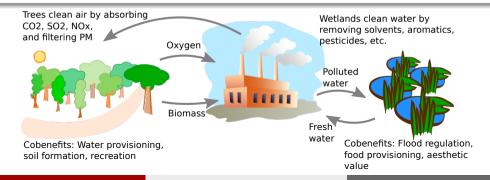
- Nature-Positive for addressing ecological degradation
 - Loss of biodiversity, ecosystem goods and services

- Socially Just for addressing social inequities
 - Shortfalls in human well-being

Eco-Synergy: Engineering and Ecosystems

How does industry depend on ecosystems?

- Source of goods like water, minerals, biomass
- Sink for wastes to air, water, land
- Services that support industrial activities such as air and water quality regulation, food and water provisioning





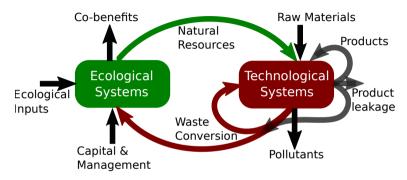
• Eco-efficiency, life cycle design

Bakshi, Ziv, Lepech, Env. Sci. Technol., 2015



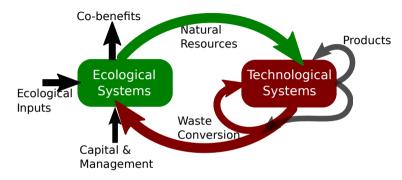
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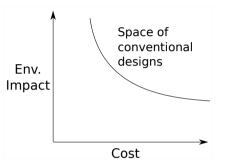


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- Techno-ecological synergy
- Sustainable TES

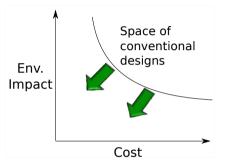
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- Watershed management (Lee et al., 2021)
- Agricultural landscape design and FEW nexus (Hanes et al., 2017, 2018)
- Single-family home and yard (Urban and Bakshi, 2013)
- 20,000 US manufacturing sites (Gopalakrishnan et al., 2019a)
- Point and non-point source emissions in US counties (Gopalakrishnan et al., 2019b)
- Ecosystem services in Life Cycle Assessment (Liu and Bakshi, 2018, 2019)

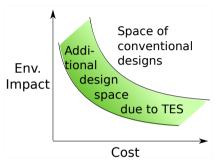
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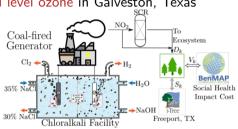


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Goal: Manufacture chlorine and manage ground level ozone in Galveston, Texas **Objectives**

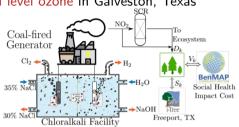
Decision variables



Goal: Manufacture chlorine and manage ground level ozone in Galveston, Texas **Objectives**

• Minimize (Cost of production) and (Cost to society)

Decision variables



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Decision variables

- SCR size
- Reforestation area
- Chlorine production rate



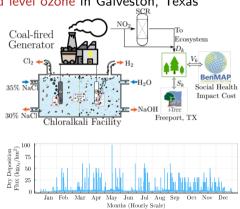
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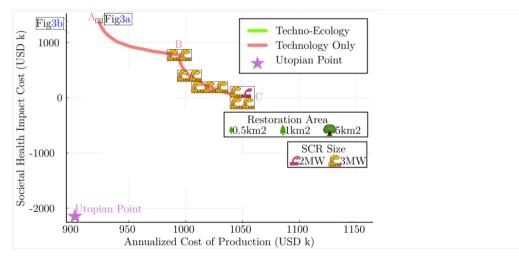
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- Air quality constraints
- Vegetation growth dynamics (FVS)
- Pollution uptake by vegetation (iTree)
- Chloralkali process model (Otashu and Baldea, 2019)

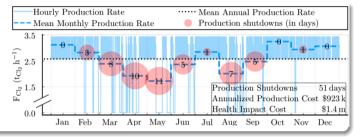


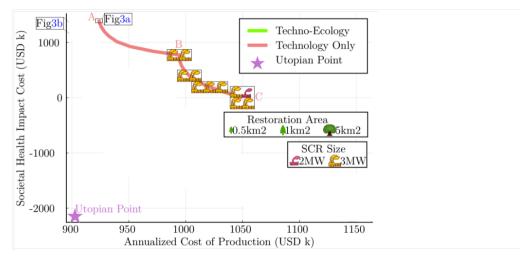


(Shah and Bakshi, ACS SCE, 2021)

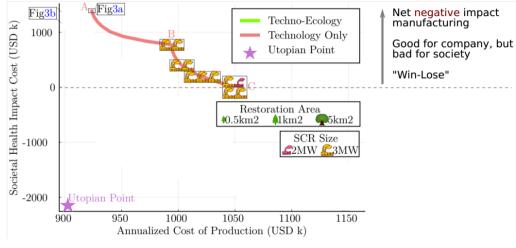
Dynamic TES Design and Operation of Chlor-Alkali Process

- Technology only
- Minimum production cost

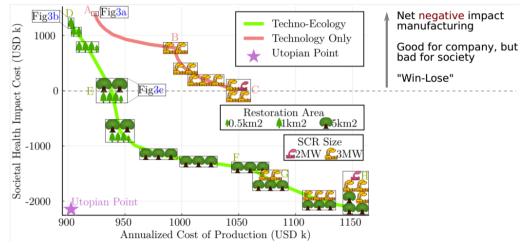




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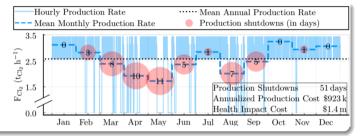
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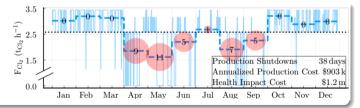
⁽Shah and Bakshi, ACS SCE, 2021)

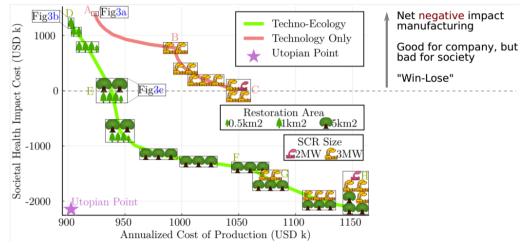
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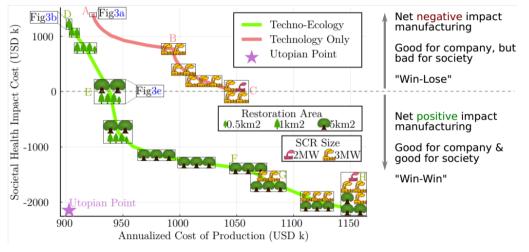


- Techno-Ecological Synergy
- Minimum production cost
- Win-win solution





⁽Shah and Bakshi, ACS SCE, 2021)



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Seeking Synergies with Nature

Nature-positive design

Synergies with nature can provide net-positive designs and innovative solutions

Seeking Synergies with Nature

Nature-positive design

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Opportunities from Eco-Synergy

By 2030, nature-positive and society-positive businesses are expected to provide

- \$10 trillion of business opportunities
- 395 million jobs

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Synergies with nature can provide net-positive designs and innovative solutions

Opportunities from Eco-Synergy

By 2030, nature-positive and society-positive businesses are expected to provide

- \$10 trillion of business opportunities
- 395 million jobs

Forward-looking businesses are figuring out how to develop such synergies and **benefit** from them

(World Economic Forum, New Nature Economy Report II, 2020)

Conclusions

- Urgent solutions are needed for addressing,
 - Climate change: Net-zero GHG emissions by 2050
 - Ecological degradation: Nature-positive business decisions
 - Social inequities: Socially just decisions
- Small tweaks to the existing system such as increasing efficiency, using renewable energy, or reducing life cycle impact will not be enough
- Real progress requires reinvention of the CMI and shift of the engineering paradigm
 - Net-zero requires reinvention of CMI as a circular enterprise
 - Nature-positive requires shifting the engineering paradigm to accounting for nature and respecting its limits
- Need systematic methods and tools for addressing the challenges

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