Mapping the Path to a Net-Zero Chemicals Industry by Long-Term Planning with Changes in Technologies and Climate

Vyom Thakker[1] and Bhavik Bakshi[1]

[1]The Ohio State University

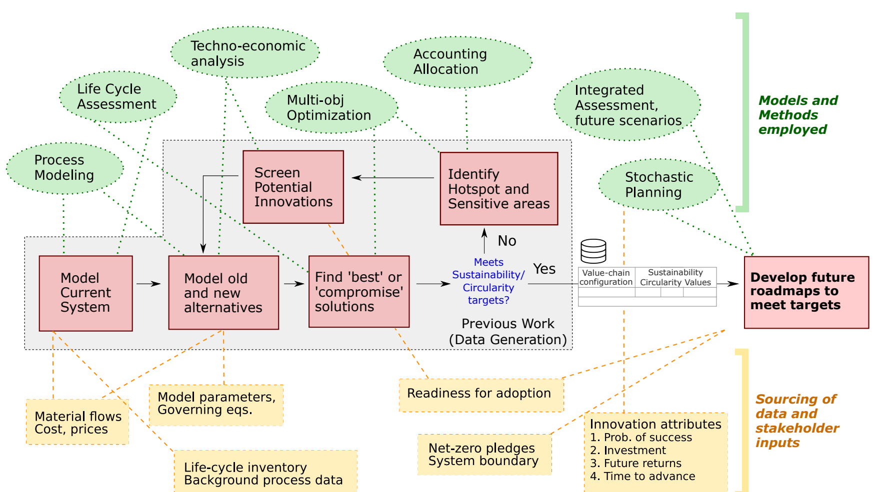
September 18, 2023

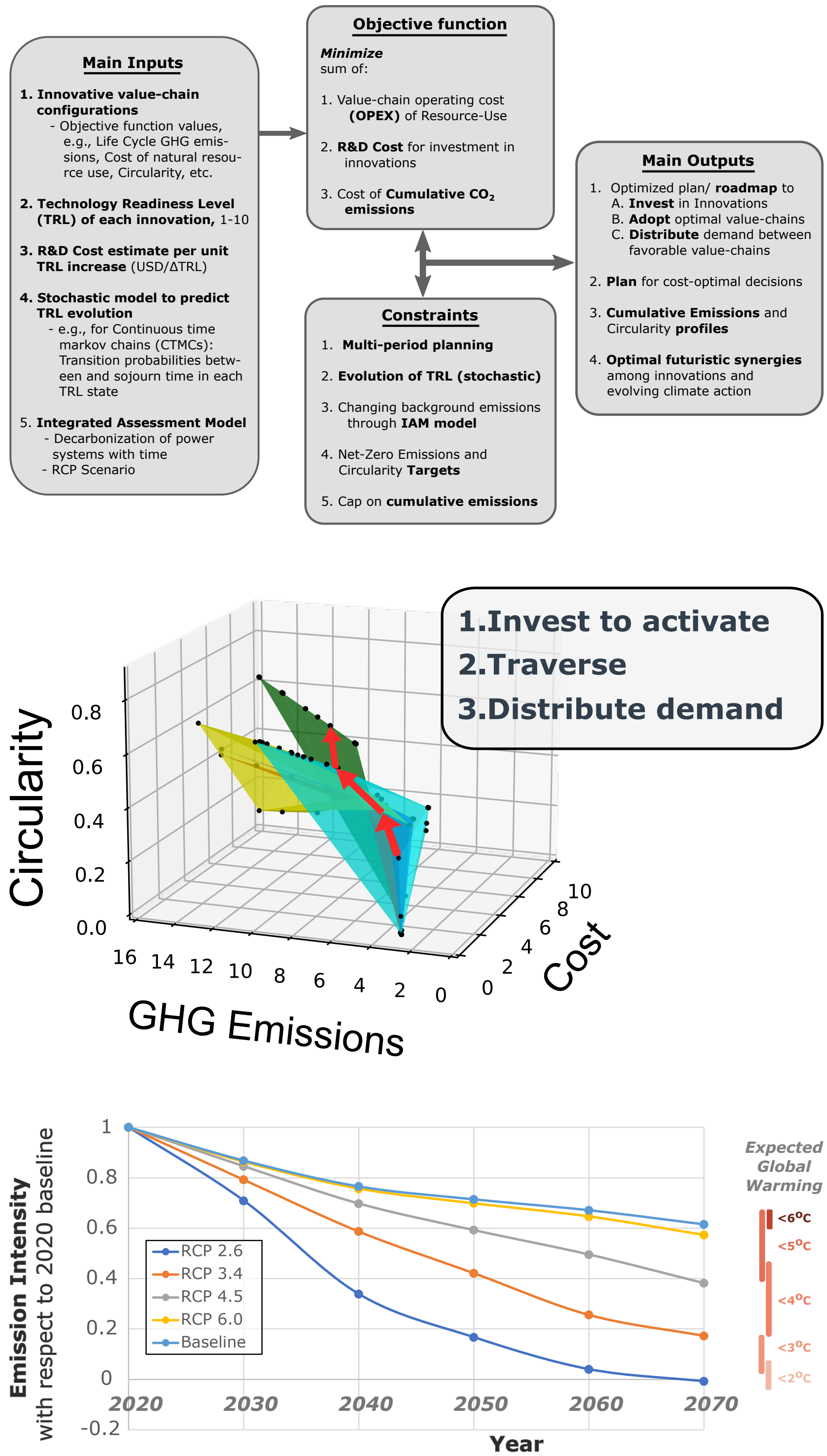
Abstract

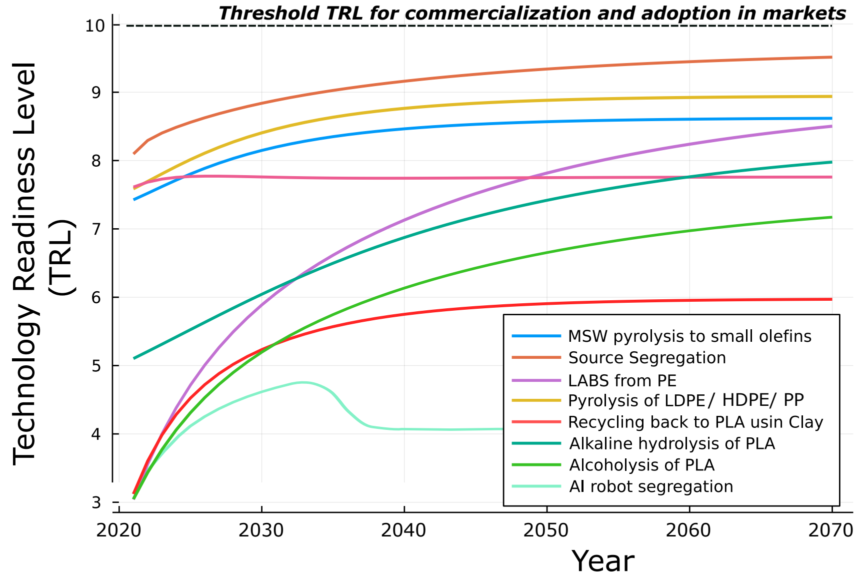
Many corporations and nations have pledged to reach net-zero emissions within a few decades. Meeting such targets for greenhouse gases, plastics, etc. requires systematic methods to guide investment in technologies and value-chain alternatives, and develop roadmaps. The proposed framework is a multi-period planning model to guide optimal reforms in cradle-to-cradle life-cycle networks across the time horizon. It aims to meet environmental targets while minimizing the total annualized marginal cost of natural resources and the investment cost associated with adoption of novel technologies. This considers the evolution of technology readiness levels as S-curves or continuous time Markov-chains. Integrated Assessment models account for climate change, decarbonization due to energy mix changes, and carbon taxes. Multiple climate change scenarios and shared socioeconomic pathways are used to model the future. In addition to providing roadmaps, the outputs can also be used to identify technologies that will be robust to future scenarios.

Hosted file

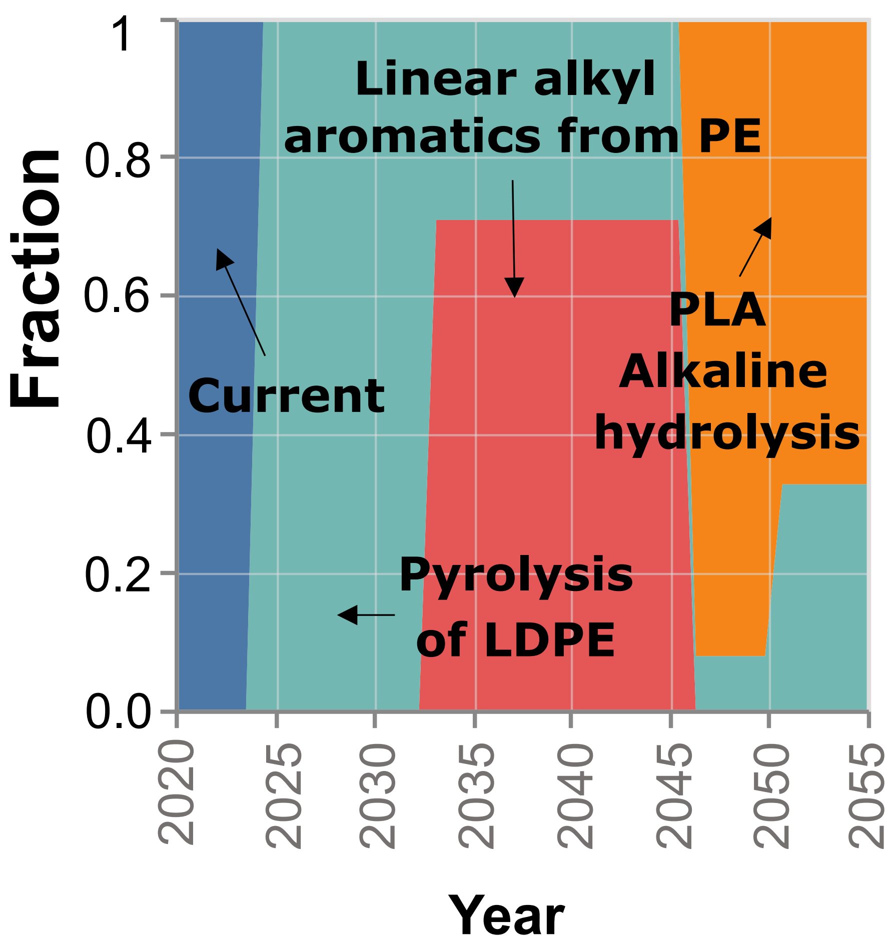
`roadmap-toy_d3.tex` available at https://authorea.com/users/665741/articles/666797-mapping-the-path-to-a-net-zero-chemicals-industry-by-long-term-planning-with-changes-in-technologies-and-climate



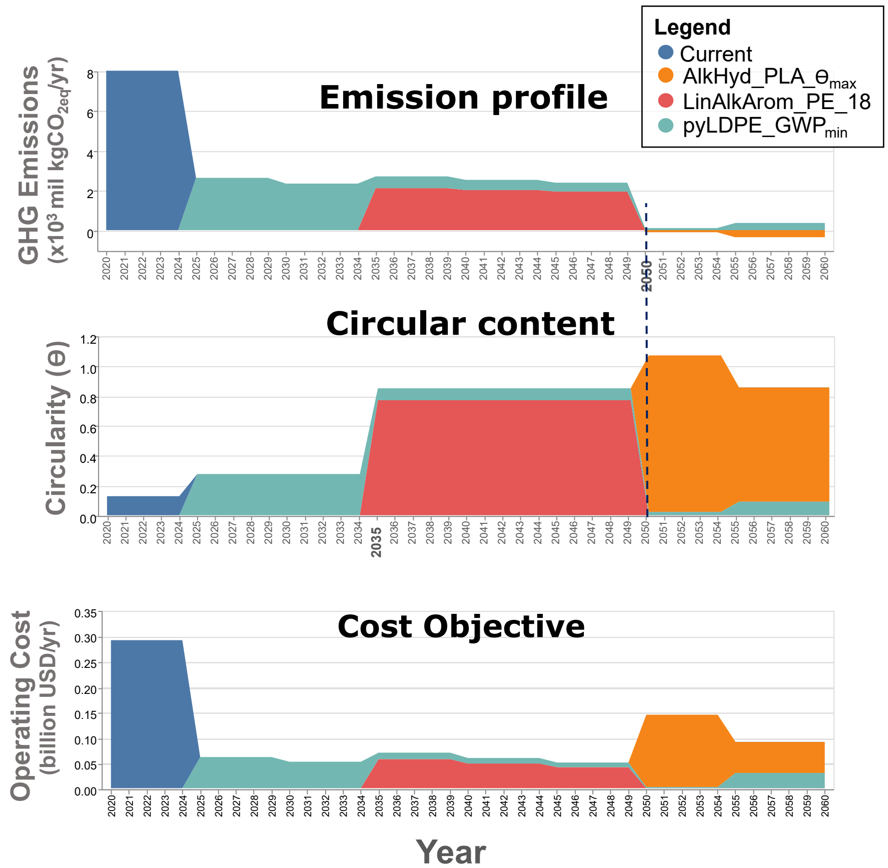

Main Inputs
1. Innovative value-chain configurations
- Objective function values, e.g., Life Cycle GHG emissions, Cost of natural resource use, Circularity, etc.
2. Technology Readiness Level (TRL) of each innovation, 1-10
3. R&D Cost estimate per unit TRL increase (USD/ΔTRL)
4. Stochastic model to predict TRL evolution
- e.g., for Continuous time markov chains (CTMCs): Transition probabilities between and sojourn time in each TRL state
5. Integrated Assessment Model
- Decarbonization of power systems with time
- RCP Scenario
Objective function
Minimize
sum of:
1. Value-chain operating cost (OPEX) of Resource-Use
2. R&D Cost for investment in innovations
3. Cost of Cumulative CO_2 emissions
Constraints
1. Multi-period planning
2. Evolution of TRL (stochastic)
3. Changing background emissions through IAM model
4. Net-Zero Emissions and Circularity Targets
5. Cap on cumulative emissions
Main Outputs
1. Optimized plan/ roadmap to
A. Invest in Innovations
B. Adopt optimal value-chains
C. Distribute demand between favorable value-chains
2. Plan for cost-optimal decisions
3. Cumulative Emissions and Circularity profiles
4. Optimal futuristic synergies among innovations and evolving climate action
1.Invest to activate
2.Traverse
3.Distribute demand
Circularity
0.0
0.2
0.4
0.6
0.8
GHG Emissions
16
14
12
10
8
6
4
2
0
Cost
0
2
4
6
8
10
Emission Intensity
with respect to 2020 baseline
1
0.8
0.6
0.4
0.2
0
-0.2
2020
2030
2040
2050
2060
2070
Year
RCP 2.6
RCP 3.4
RCP 4.5
RCP 6.0
Baseline
Expected Global Warming
<6°C
<5°C
<4°C
<3°C
<2°C



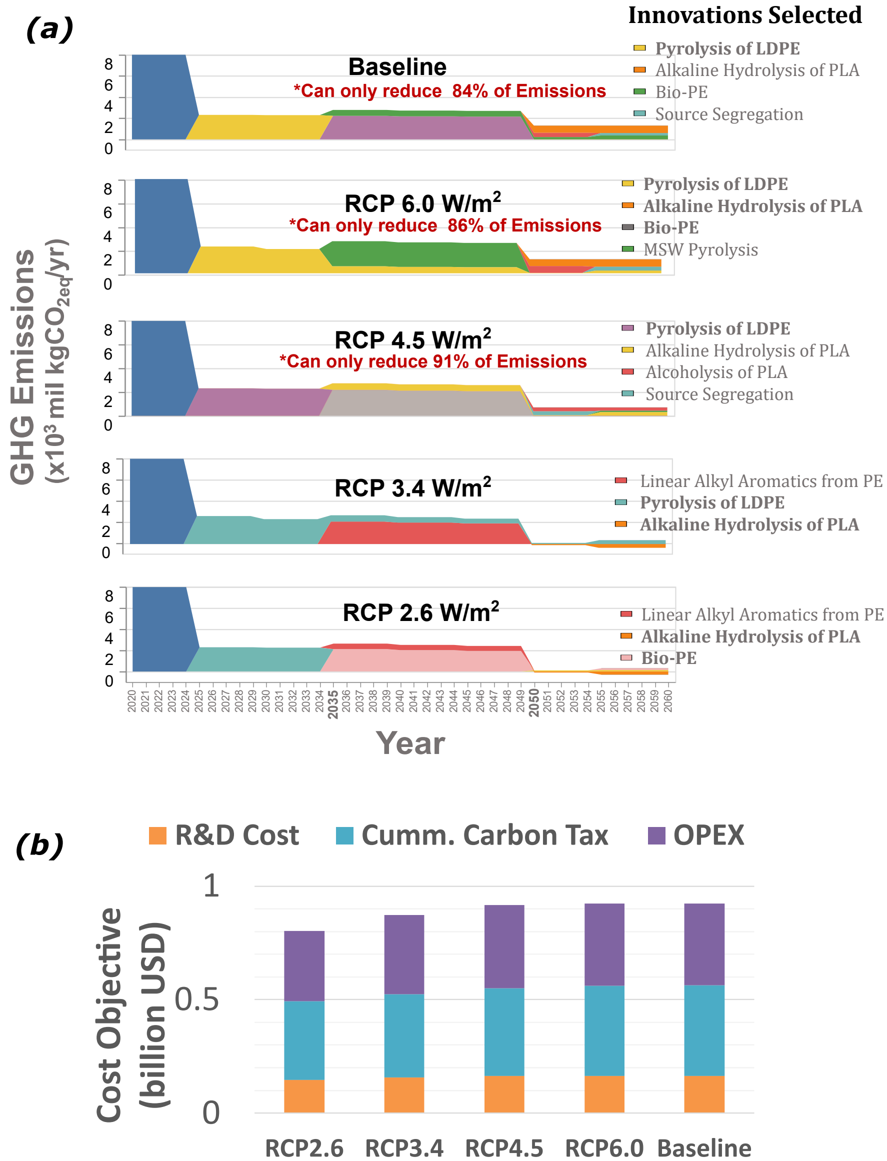
Threshold TRL for commercialization and adoption in markets
Technology Readiness Level (TRL)
Year
MSW pyrolysis to small olefins
Source Segregation
LABS from PE
Pyrolysis of LDPE/ HDPE/ PP
Recycling back to PLA usin Clay
Alkaline hydrolysis of PLA
Alcoholysis of PLA
AI robot segregation



Linear alkyl aromatics from PE
Current
PLA Alkaline hydrolysis
Pyrolysis of LDPE
Fraction
Year



Legend
Current
AlkHyd_PLA_θmax
LinAlkArom_PE_18
pyLDPE_GWPmin
Emission profile
GHG Emissions
(x10³ mil kgCO2eq/yr)
Circular content
Circularity (θ)
Cost Objective
Operating Cost
(billion USD/yr)
Year


(a)
Innovations Selected
Baseline
*Can only reduce 84% of Emissions
Pyrolysis of LDPE
Alkaline Hydrolysis of PLA
Bio-PE
Source Segregation
RCP 6.0 W/m2
*Can only reduce 86% of Emissions
Pyrolysis of LDPE
Alkaline Hydrolysis of PLA
Bio-PE
MSW Pyrolysis
RCP 4.5 W/m2
*Can only reduce 91% of Emissions
Pyrolysis of LDPE
Alkaline Hydrolysis of PLA
Alcoholysis of PLA
Source Segregation
RCP 3.4 W/m2
Linear Alkyl Aromatics from PE
Pyrolysis of LDPE
Alkaline Hydrolysis of PLA
RCP 2.6 W/m2
Linear Alkyl Aromatics from PE
Alkaline Hydrolysis of PLA
Bio-PE
GHG Emissions
(x10^3 mil kgCO2eq/yr)
Year
(b)
R&D Cost
Cumm. Carbon Tax
OPEX
Cost Objective
(billion USD)
RCP2.6
RCP3.4
RCP4.5
RCP6.0
Baseline

Mapping the Path to a Net-Zero Chemicals Industry by Long-Term Planning with Changes in Technologies and Climate

Journal:	*AIChE Journal*
Manuscript ID	AIChE-23-26386
Wiley - Manuscript type:	Research Article
Date Submitted by the Author:	17-Sep-2023
Complete List of Authors:	Thakker, Vyom; The Ohio State University, Department of Chemical Engineering; The Dow Chemical Company Bakshi, Bhavik; The Ohio State University, Department of Chemical and Biomolecular Engineering; Arizona State University, College of Global Futures
Keywords:	Multi-period Planning, Carbon Neutrality, Circular Economy, Life Cycle Assessment, Climate change

Mapping the Path to a Net-Zero Chemicals Industry by Long-Term Planning with Changes in Technologies and Climate

Vyom Thakker[1,2] and Bhavik R. Bakshi*[1,3]

[1]William G. Lowrie Department of Chemical and Biomolecular Engineering, , The Ohio State University, Columbus, Ohio 43210, USA

[2]Present Address: Machine Learning, Optimization and Statistics, Core R&D, The Dow Chemical Company, Lake Jackson, TX, 77566, USA

[3]College of Global Futures, Arizona State University, Tempe, Arizona 85287, USA

Abstract

Many corporations and nations have pledged to reach net-zero emissions within a few decades. Meeting such targets for greenhouse gases, plastics, etc. requires systematic methods to guide investment in technologies and value-chain alternatives, and develop roadmaps. The proposed framework is a multi-period planning model to guide optimal reforms in cradle-to-cradle life-cycle networks across the time horizon. It aims to meet environmental targets while minimizing the total annualized marginal cost of natural resources and the investment cost associated with adoption of novel technologies. This considers the evolution of technology readiness levels as S-curves or continuous time Markov-chains. Integrated Assessment models account for climate change, decarbonization due to energy mix changes, and carbon

*Corresponding Author: B.R. Bakshi (Bhavik.Bakshi@osu.edu)

taxes. Multiple climate change scenarios and shared socioeconomic pathways are used to model the future. In addition to providing roadmaps, the outputs can also be used to identify technologies that will be robust to future scenarios.

Keywords: Multi-period Planning, Carbon Neutrality, Circular Economy, Life Cycle Assessment, Integrated Assessment Models, Technology Evolution, Climate Change Policy

1 Introduction

Increasing impact of human activities on Earth's ecosystem goods and services, has brought us to a new geological epoch, called the Anthropocene.[1] If these trends of ecological degradation by natural resource exploitation and environmental pollution continue, Earth will cross the tipping points for environmental sustenance and exit the safe-operating-space[2] for human well-being. To avoid and mitigate these adverse outcomes, the world collectively needs new technologies, policies and supply-chains to facilitate sustainability transitions to an economy with Net-zero emissions and recycling of waste.[3,4] Therefore, modeling and optimizing the implementation of sustainability transitions is a subject of growing interest in academia, policy-making and corporate R&D. Several organizations have pledged to achieve net-zero emissions and high sustainable content in their products for as early as 2030. These include carbon neutrality targets set by governments according to the Paris Accord;[5] organizational net-zero emission targets for 2030 (by Apple, Alphabet, Microsoft, Walgreens, Kroger, etc.), 2040 (by Walmart, Amazon, Target, Intel, FedEx, Pepsico, etc.) and 2050 (by ExxonMobil, BP, Dow Chemical, Mitsubishi, etc.);[6,7] and circularity targets by signatories of the Plastics Pact.[8] Actions and interventions towards achieving these net-zero emissions and circularity targets present a rare opportunity to not only achieve environmental sustainability but simultaneously encourage ecosystem restoration and protection, address social inequities. If done right, this can provide companies with the benefits of market leadership through innovation.

Meeting these challenges requires adoption of a trans-disciplinary or convergent systems view to guide future developments, including approaches for developing integrated value-chain and supply-chain networks. This alludes to an immediate need for (1) evaluating the performance of each organization from a holistic perspective, and (2) for creating tools that facilitate transitions and build roadmaps towards achieving these targets. Despite ambiguous reporting mechanisms and system boundaries for many of these targets, several standards and initiatives such as Science Based Targets Initiative (SBTi), Task Force for Climate-related Finance Disclosures (TCFD) and International Sustainability & Carbon Certification (ISCC) are being developed and implemented. However, current literature and corporate intellectual property lack a concrete framework to guide these transitions holistically and find optimal roadmaps to invest in novel technologies and partnerships. A lot of current work[9] is based on building localized models for targeted use-cases, such as displacement of vendors in a supply-chain network or a singular change of operations on the company's economic performance. Kohler et al (2019)[10] identify the state of the art methods and theories being proposed with regards to these transitions. These include theoretical frameworks that borrow concepts from evolutionary economics, sociology and institutional dynamics, examples of which are Transition Management framework, Multi-Level Perspective (MLP), Strategic Niche Management framework, etc. These sophisticated methods study the substitution dynamics and reorientation trajectories of innovative product systems. However, these concern themselves with adoption of singular innovations, often missing out on synergistic effects and implications on environmental impact of the entire system. Kohler et al. (2019) also identify this short-coming in recent literature, suggesting that novel frameworks are needed which allow selection and planning of innovations based on holistic environmental impact and potential synergies with conventional systems currently in place and other innovations being proposed. In the operations management and ecological economics domains, portfolio management approaches to predict the odds of technology adoption are commonly described based on heuristics[11,12] and market indicators,[13] and often lack the holistic environmental impact assessment for prioritization of investments. Another body of academic literature focuses on evaluation of novel technologies and product system in a futuristic context with marginal supply mixes of electricity, while calculating the holistic environmental impact using consequential life cycle assessment approaches.[14] However, these articles do not extend their scope to include multiple alternatives and perform planning to generate temporal roadmaps for the future. Little to no work has been done on guiding and planning the adoption of novel solutions to meet the ambitious targets to battle climate change and pollution. Particularly, adoption plans must account for climate change phenomena such as evolving energy mix and policy towards decarbonization. These efforts must leverage Integrated Assessment Models which characterize global environmental change through quantification of interactions between human and earth systems.[15]

In this manuscript, we develop a roadmapping framework that builds upon previous work to design sustainable circular economies[16,17] and utilizes concepts from process systems engineering such as superstructure optimization and multi-period planning[18,19] to identify optimal transition strategies to meet environmental targets. The roadmapping framework involves selection of innovative value-chain solutions at different time-periods to always meet consumer demand, while achieving the overall targets for life cycle environmental emissions in the future. The solutions minimize investment costs by capturing the evolution of technology readiness levels (TRLs) in the future through stochastic processes. The framework also allows the setting of carbon caps or taxation to ensure that the solution does not emit unfavorably in the duration leading to the targets being met. The total life cycle emissions change along the time horizon due to upstream decarbonization and climate change policy, accounted for, using Integrated Assessment Models (IAMs).

The manuscript is organized as follows. The next section describes the methods employed to develop roadmaps to meet emissions and circularity targets. This includes a brief description of previously developed multi-objective life-cycle optimization toolkits,[17,20] which can be used to generate data to be used as input for the framework proposed in this manuscript. Alternatively, users of the proposed framework can also feed data corresponding to key value-chain configurations of interest for road-mapping to meet their targets. The method section then describes the key elements of the road-

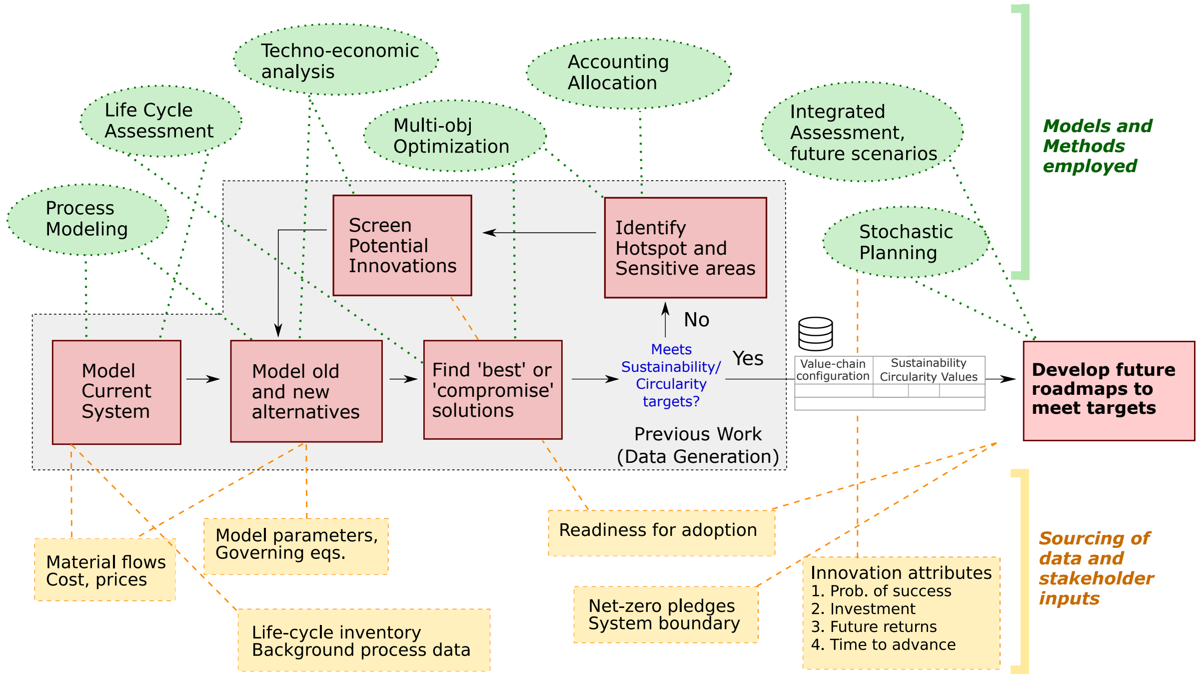


Figure 1: Proposed workflow to efficiently integrate design of conventional and innovative value-chains for generating roadmaps to meet environmental targets towards sustainable circular economy.

mapping framework in sections 2.1 - 2.5. Next, the case study section describes the problem statement for identifying optimal roadmaps for innovations and climate action in the packaging industry for carbon-neutral and circular value-chains of grocery bags. Finally, the results and discussion section provides insights on the general applicability of the road-mapping framework and findings from applying it to the case study.

2 Method

The novel roadmapping framework developed in this manuscript is intended to design strategies to invest in and adopt innovations and interventions in life-cycle networks of products, which can ensure that environmental targets of sustainability and circularity are met while satisfying stakeholder objectives such as cost and cumulative life-cycle environmental impact in the selected time horizon. The inputs consist of the emissions, circularity and cost metrics for multiple value-chain configurations after introduction of each innovation. The outcome is a roadmap or plan for investment and adoption of optimal innovations at different time-points based on sustainability targets, technology evolution, integrated assessment models for climate change and carbon taxation. Capturing the dynamics of how technologies are likely to evolve in terms of their readiness for adoption and the imminent decarbonization of several activities beyond the influence of a stakeholder is expected to yield holistically guided roadmaps for transitioning towards net-zero emissions and circularity.

Data Generation and Consolidation

While it is recommended to follow the strategy and modeling techniques from previously developed methods to generate data for the proposed framework (figure 1), users can also use their own input dataset which has to contain the sustainability and circularity metrics for innovative value-chain configurations. Using the proposed workflow from figure 1 would ensure building well-informed roadmaps with carefully screened innovations and with due consideration given to trade-offs between circularity, greenhouse gas emissions and costs. Each of the steps in the figure (red boxes), except 'Develop a roadmap' corresponds to an open-source framework developed and published, with the following objectives.

1. Model available alternatives: Designing conventional value-chains by optimizing cradle-to-cradle life-cycle networks of a consumer product.[20] To reduce the chance of the proposed strategies causing shifting of environmental burdens to other parts of the value-chain, we rely on life cycle assessments to quantify the environmental impacts from the entire life-cycle of current and emerging solutions, ranging from raw material extraction, manufacturing, processing, transport, usage, end-of-life and recycling.[21]

2. Identify best pathways: Obtaining Pareto fronts to quantify trade-offs between objectives such as Sustainable Circular Economy (SCE), namely Circularity, Global Warming Potential (GWP) of greenhouse-gas emissions, and cost of natural resource use.[16] Circularity is defined as the ratio of regenerated value through circular flows

and the value of manufactured materials. Depending on the measure used for quantifying value (money or bio-degradable mass), circularity can be defined in monetary or ecological terms. GWP and natural resource use are calculated using a life cycle system boundary and ReCiPe impact assessment factors[22] to calculate GWP from value-chain emissions in kgCO2 equivalents. While this manuscript utilizes monetary circularity (θ) and GWP for target-setting in roadmaps, it can easily be replaced by a definition of user's preference in the input data-set.

3. Identify hotspot and sensitive areas: Screening of large list of new technologies, supply-chain strategies, policies, etc. based on sectors which are emission hotspots and model parameters which can have optimal perturbations to best improve SCE objectives.[23]

4. Identify potential innovations: Ranking of selected alternatives, and generation of Pareto-fronts corresponding to each alternative.[17]

Once a selected subset of innovations is included in the life-cycle network, several Pareto-fronts can be obtained for each innovation or combinations of those innovations which are expected to show a synergistic effect. However, in order to create a roadmap to SCE, the questions corresponding to what, when and how to invest and adopt these value-chain solutions need to be answered. The roadmapping framework developed in the paper aims to accomplish this by developing a sophisticated multi-period planning framework. The schematic for all the processes involved to design roadmaps for SCE and to meet environmental targets is demonstrated in figure 1.

The following sub-sections describe the math corresponding to each of the components within the framework, as depicted in figure 2, including the long-term planning method, stochastic evolution of technology readiness levels, accounting for upstream decarbonization through IAMs and carbon budget utilization. The case-study section will describe the implementation of these components for a case study on packaging innovations to have grocery bags value-chains with net-zero emissions and high circularity.

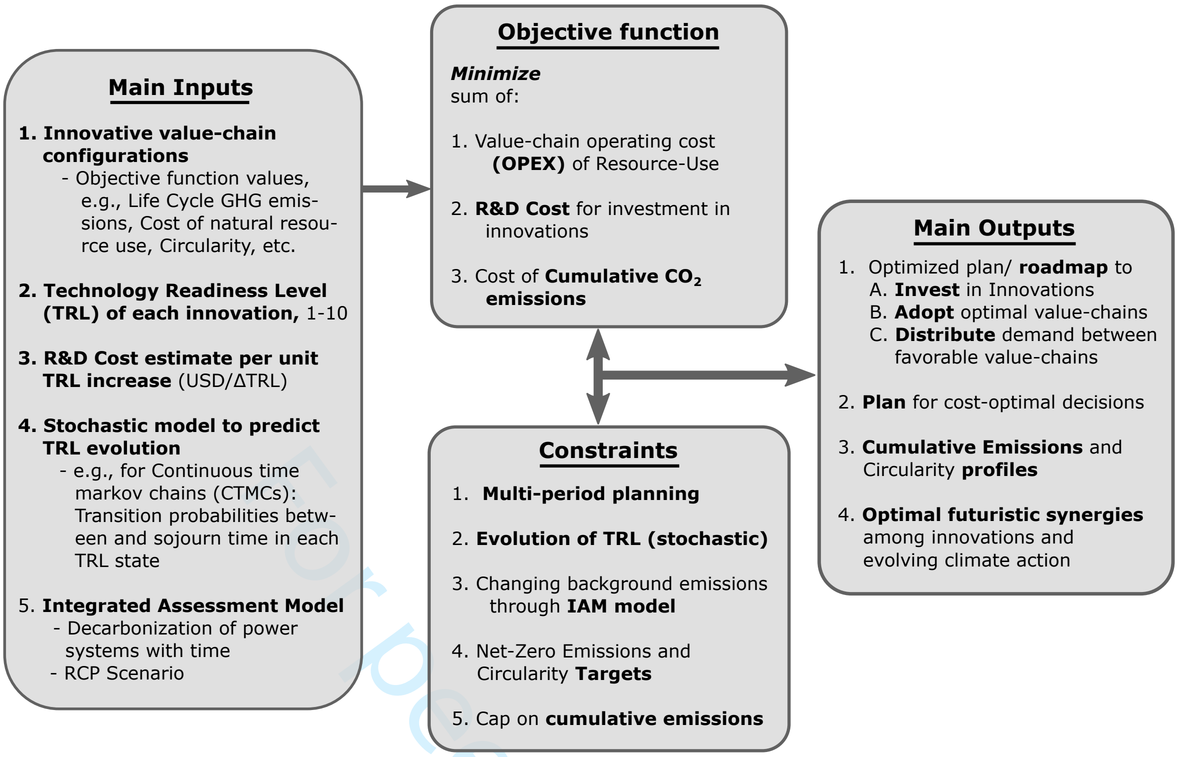


Figure 2: Summary of the Multi-period planning framework to roadmap innovations for meeting net-zero emissions and circularity targets. Notably, the most important input data required are the multiple sets (for each innovation) of the values of objectives such as life-cycle impact (e.g., greenhouse gas emissions), circularity and cost for one or more value-chain configurations with the innovation. Ideally, these sets should be found through the proposed strategy in figure 1, i.e. through multi-objective optimization of life-cycle networks using previously developed open-source frameworks.

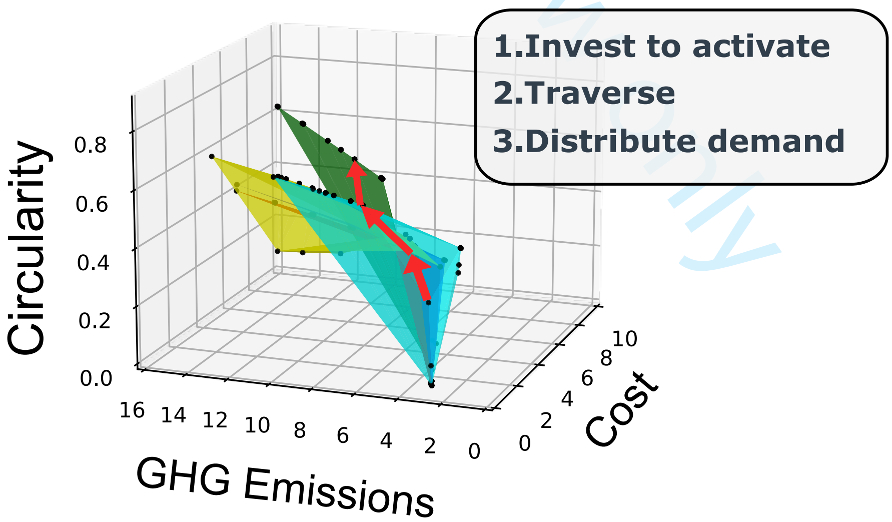


Figure 3: Pareto-fronts for available innovations; The multi-period planning framework selects which innovations to invest in during each time period, and ultimately how to distribute the consumer demand (functional unit) between various compromise solutions on the Pareto-fronts. Each point corresponds to a value-chain solution scaled according to the volume carrying capacity of a single household. GHG emissions are expressed in $kgCO_2$ equivalents, and Cost is estimated using the price of natural resources in USD.

2.1 Multi-period Planning formulation

This section describes the general multi-period planning constraints, denoted as f_1 in equation 1. These constraints represent the basis for making planning decisions depicted in figure 3, and are described below.

- Which **innovations** to choose for **investment** and when?
- If invested in, which **compromise solution** on the Pareto-front corresponding to the chosen innovation to **select for adoption** and when?
- If multiple compromise solutions are favorable, how to **distribute consumer demand** among favorable compromise solutions?

The decision variables of the planning problem which capture the above choices are as follows.

- Whether an investment is made in the innovation i within the time period τ, $y_{i\tau} \in \mathbb{B}$.
- Whether a compromise value-chain solution $k \in \mathbb{K}_i$ on the innovative Pareto-front corresponding to ith innovation is chosen to satisfy consumer demand in time period τ, $y_{k\tau} \in \mathbb{B}$. The greenhouse gas (GHG) emissions from each value-chain solution is recorded in the parameter Em_k and circularity is measured in terms of monetary regeneration factor and is recorded as θ_k.
- Fraction of consumer demand satisfied by a compromise value-chain solution (k) in time period τ, $x_{k\tau} \in \mathbb{R}$

The overall optimization formulation for the roadmapping framework depicted in figure 2 consists of the objective functions computed from decision variables, and corresponding constraints on these variables to capture technology readiness evolution, changing upstream emissions and targets.

$$\min_{\substack{y_{i\tau},t_{i\tau}\\x_{k\tau},y_{k\tau},t_{k\tau}}} z := \sum_{\tau\in\mathbb{T}}\left[\sum_{k\in\mathbb{K}_i}\text{OPEX}_k + \sum_{i\in\mathbb{I}}\text{R\&D Cost}_i\left\{RL_{\max} - \mathbb{E}\left[RL_i\right]\right\}\right] + \text{Carbon Tax}$$

$$\begin{aligned}
\text{s.t.}\quad & f_1(x,y,t)\geq 0, && \textbf{Multi-Period Planning Constraints}\\
& RL_i = f_2^i(t_i,\cdot)\geq 0 && \textbf{Evolution of Innovation TRLs}\\
& A(t_k) = f_3^k\left(A_0,\text{RCP}_{rf},t_k\right) && \textbf{Integrated Assessment Models}\\
& \text{GHG}\left(x,y,t^{\text{GHG}=0}\right)\leq 0 && \textbf{Climate Change Target}\\
& \text{Circularity}\left(x,y,t^{\theta\geq\theta^*}\right)\geq 1.0 && \textbf{US Plastics Pact Target}\\
& \sum_{k,\tau} f_4\left(x_k,t_k,A(t_k)\right)\leq B && \textbf{Cumulative CO}_2\textbf{ emissions cap}\\
& y_{i\tau},\ y_{k\tau}\in\mathbb{Z}\in\{0,1\}\\
& x_{k\tau} = \mathbb{R}\in[0,1]\\
& t_{i\tau},\ t_{k\tau}\in\mathbb{R},\tau\in\mathbb{Z}=\{1..7\}
\end{aligned}\tag{1}$$

In order to ensure proper allocation of resources and define time periods of availability of innovations, the following structural constraints are added upon the decision variables.

1. Once an innovation is invested in during a time period, it is activated and made available for all time periods following this time period.

$$y_{i(\tau+1)}\geq y_{i\tau}\quad\forall\ i\in\mathbb{I},\ \tau\in\{1..N-1\}\tag{2}$$

2. After investment in an innovation (i), all the value-chain solutions on the corresponding Pareto-front ($k\in\mathbb{K}_i$) become available for adoption. Only one such Pareto-optimal (or compromise) solution is chosen in a particular time period for adoption.

$$\sum_{k\in\mathbb{K}_i} y_{k\tau}\leq y_{i\tau}\quad\forall\ i\in\mathbb{I},\ \tau\in\{1..N\}\tag{3}$$

3. If a Pareto-optimal solution (k) is chosen for adoption, the planning framework can

distribute the consumer demand (or functional unit) between all the chosen options. This is denoted using a continuous variable bound between $[0, 1]$, which is non-zero for k only if it is chosen for adoption.

$$\begin{aligned} y_{k\tau} \geq x_{k\tau} \quad \forall\, k \in \mathbb{K},\ \tau \in \{1..N\} \\ 0 \leq x_{k\tau} \leq 1, \mathbb{R} \end{aligned} \tag{4}$$

4. Selection of a Pareto-optimal solution (k) on a Pareto-front corresponding to the innovation i can happen only after investment is made in i.

$$\sum_{k \in \mathbb{K}_i} t_{k\tau} \geq t_{i\tau} \quad \forall\, i \in \mathbb{I},\ \tau \in \{1..N\} \tag{5}$$

5. If an investment is made in an innovation i during a time period τ, value of the continuous variable $t_{i\tau}$, indicating the time of investment, is allowed to be between 0 and (TH/N). Here TH denotes the entire time horizon duration and N denotes the number of time periods considered. This is ensured by imposing the following constraint.

$$\begin{aligned} (\mathrm{TH}\,/N) y_{i\tau} \geq t_{i\tau} \quad \forall\, i \in \mathbb{I},\ \tau \in \{1\} \\ (\mathrm{TH}\,/N) \left[y_{i\tau} - y_{i(\tau-1)} \right] \geq t_{i\tau} \quad \forall\, i \in \mathbb{I},\ \tau \in \{2..N\} \end{aligned} \tag{6}$$

Notably, these constraints are valid across multiple time periods in the time horizon, with few continuity and inventory type constraints to ensure all investment in innovations results in future availability of value-chain solutions corresponding to the invested innovations. In a way, this choice can be understood as traversal from one innovative Pareto-front to the other in the objective domain, across different time periods as shown in Figure 3.

2.2 Evolution of Eco-innovations

One of the major short-comings of recent research on planning for climate action ignores the dynamic nature of each innovation's readiness for adoption. This would have a major effect in estimating when it would become available for adoption in the network. The framework proposed in this manuscript captures this attribute within the planning optimization methodology. The investment needed in the innovation at any time is assumed to be directly proportional to how far the RL of an innovation at that time is from the RL corresponding to the diffusion stage (RL_{max}). The RL of an innovation is modeled either deterministically or stochastically as a function of time, as described in detail in this section. Therefore, as the RL evolves over time, the cost needed to bring the innovation close to adoption changes too. Additionally, an investment is needed to make all the Pareto-optimal solutions on the innovative Pareto-front available for adoption, so as to meet the climate change and circularity targets set by the user. Thus, evolution of RL of innovations is important for multiple reasons within the planning framework. Regardless of how one chooses to model this evolution, for solving the optimization problem, we propose to surrogate these usually non-linear evolution profiles using piecewise linear functions for easier integration with the multi-period planning constraints.

2.2.1 S-curves (deterministic)

Typically, consulting firms and venture capitalists use learning curves,[24] experience curves[25,26] and S-curves[27] to estimate the cost and maturity of new ventures, technologies and programs. These are deterministic curves which depend on few parameters defined by experts and stakeholders. For instance, Google Circularity Gap report[28] alludes to using S-curve methodology to estimate market penetration of Circular Economy related innovations. The report quantifies the market penetration as follows.

$$y = y_0 + \frac{1}{1 + e^{-c(t-t_0)}} \tag{7}$$

Here, t_0, y_0 denote the initial values of time and market share, and the coefficient c is found using a scoring method, given to experts. The score is found using the number of competing technologies, stakeholder groups needed and disruption of current technologies. These curves can be considered as heuristics to model evolution of technology readiness levels of all innovations, which will be surrogate using piecewise linear functions and added to the planning optimization framework. While this is a simpler approach with lower need for user parameters (3 scores), it is limited in terms of the behavior it can model (only sigmoidal).

2.2.2 Options theory and Portfolio management approaches

Many approaches to find optimal portfolio strategies have been developed in recent literature, with applications to pharmaceutical and consumer goods industry. While some of these approaches are based on heuristics and market surveys, others are more quantitative and mathematically rigorous. Trade-offs between higher rigor and number of required parameters to be estimated is observed, as described in the previous section. For instance, Rogers et al. (2002)[29] propose a framework to create a roadmap for drug development in a pharmaceutical company through different TRL stages while allowing decision continuation/ abandonment and considering market risk. While we believe this rigorous approach is extremely useful and robust, it requires a large number of stakeholder inputs such as estimates of market volatility, risk-neutral probabilities, etc., and also involves complex decomposition techniques for computational tractability. We propose a simpler and less data-intensive approach to model evolution of readiness levels using Continuous-time Markov Chains (CTMC), which is needed to model diverse innovations that span across the value-chain unlike drug development specific to a single stakeholder.

2.2.3 Markov Chains (stochastic technology forecasting)

Continuous Time Markov Chains (CTMCs) are a stochastic process which can be used to model the probabilistic evolution of technology readiness levels, captured within a discrete-state space (e.g., TRL $= \mathbb{Z} \in [1, 10]$). CTMCs satisfy the Markovian property, i.e. the transition probability between state A to B at a particular time is independent how the process got to state A, and the time spent in a state (sojourn time) follows an exponential distribution. Recognizing that there are several ways to model technology forecasting, We justify the use of CTMCs for modeling Technology Readiness Levels

(TRL) over time due to the following reasons:

1. TRL can be considered as discrete states, and evolution between TRL states can be assumed to be Markovian. For instance, the probability of an innovation to transition from pilot plant state (TRL=4) to commercialization state (TRL=6) does not depend on how and when the innovation reached the pilot plant state from R&D stage.

2. Sojourn times indicate the time spent by an innovation in each state, which can be assumed to follow an exponential distribution.[30]

Since CTMCs can be viewed as a collection of independent competing exponential random variables, the next state S_c from the initial state S_a can be found as follows.

$$S_c \in argmin\{T_{ab}, b \neq a\}, \text{where } T_{ab} \sim exp(\nu_a P_{ab}), \tag{8}$$

Here ν_a is the reciprocal of the expectation of the sojourn time at state S_a, and P_{ab} indicates the probability of transition between state S_a to S_b in an embedded Discrete-time Markov Chain (DTMC). The instantaneous transition rates between any two states (q_{ab}) in a CTMC (and subsequently the rate matrix $Q = [q_{ab}]$) can therefore be found as follows.

$$q_{ab} = \begin{cases} \nu_a P_{ab}, & \text{if } a \neq b \\ -\nu_a, & \text{if } a = b \end{cases} \tag{9}$$

While the rate matrix (Q) can characterize the CTMC completely, most of the parameters that can be learnt/ estimated or provided are a) Mean of Sojourn times, and b) Transition probabilities for embedded DTMCs. Chapman-Kolmogorov forward equation can be used to derive the transient probabilities of the stochastic process to be in a particular state at time t, given the initial state S_0, which is given by,

$$P(t) = P(t = 0) \cdot e^{Qt} \tag{10}$$

The exponential of the rate matrix is difficult to calculate and compute, and there are several ways including Euler expansion to obtain approximate solution. We use the Eigen-decomposition method (if Q is diagonalizable) to express $Q = ADA^{-1}$, where $D = \text{diag}(\lambda_1, \lambda_2 ...)$ and λ's are the eigenvalues. This allows for the following simplification and Euler expansion of each of the scalars $e^{\lambda_a t}$ independently.

$$e^{Qt} = Ae^{Dt}A^{-1}, \; e^{Dt} = \text{diag}(e^{\lambda_a t}, e^{\lambda_b}t, ...) \tag{11}$$

The transient probabilities of the Markovian process being in several states $S.$ given that it is in state S_a initially can be found from the following equation.

$$P(t) = \begin{pmatrix} p_a(t) \\ p_b(t) \\ .. \\ .. \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ .. \end{pmatrix} \cdot e^{Qt} \tag{12}$$

This probability distribution $(P(t))$ can used to identify the expectation value of the CTMC state (or TRL of innovation i) at time t, using the following equation, thereby describing the expected behavior of the CTMC and the expected readiness level of innovation i at any time t.

$$\mathbb{E}[RL_i](t) = \mathbb{E}[S](t) = \sum_{s \in \text{states}} S_s p_s(t) \tag{13}$$

While these decomposition and Euler-expansion techniques make the computation/ simulation of the CTMCs much easier, these are still non-linearities which one would want to avoid in a multi-period planning optimization model described in section 2.1. In addition, since the CTMC attributes P_{ab}, ν_a, Q, etc. can be estimated beforehand, they would just be parameters in the optimization model with the states indicating the TRL of a particular innovation. Therefore, we simulate the evolution profiles of each innovation before the optimization, as shown in figure 5 for a case study. Ultimately we surrogate these temporal profiles using piecewise linear functions with optimized breakpoints and introduce these functions in the multi-period planning problem, denoted by $f_2(\cdot)$ in equation 1.

2.2.4 Practical data acquisition limitations

Data collection for certain deterministic models is much easier than stochastic counterparts mentioned in this section. However these models are usually nothing better than heuristics for specific innovations and are very sensitive to inputs from industry experts, sector of innovation, etc. Highly rigorous models such as real-options theory are great for industry-specific problems with clearly defined parameters and uncertainty. However, these are also very complex to include within the roadmapping optimization framework. While the CTMC approach counters these short-comings or incompatibilities and is promising to model technology evolution, it still requires numerous parameter inputs in the form of mean sojourn times and transition probabilities.

2.3 Integrated Assessment Models for varying background emissions

While creating roadmaps for future technologies and supply-chains, it is essential to consider practical aspects such as changing policy around environmental change and interventions in the background life cycles. Integrated assessment modeling is a sophisticated and complex branch of ecological economics, which integrates aspects from various scientific disciplines to model earth systems, human interactions and policy. It has been successfully applied to support many climate change decisions and policies, such as Millennium Ecosystem Assessment. In this manuscript, we use Integrated Assessment Models (IAMs), specifically IMAGE (Integrated Model to Assess the Global Environment),[31] developed to understand long-term impacts of global changes due to interacting socioeconomic and environmental factors. It has been used to simulate future emissions from the electricity generation sector considering (a) growth of electricity demand for various shared socioeconomic pathways (SSP 1-5), and (b) policy action to meet greenhouse gas concentration targets set according to Representative Concentration Pathways for the fol-

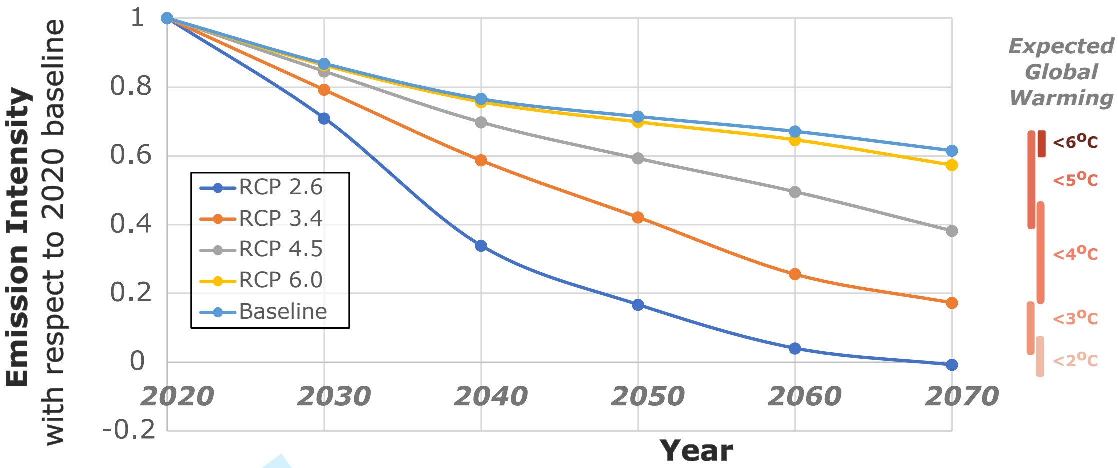


Figure 4: Emission intensity from electricity generation, projected for the USA in the future considering Middle-of-the road (SSP2) scenario, constructed using the Integrated Model to Assess the Global Environment (IMAGE) IAM model.

lowing radiative forcing values in 2050 - (RCP_{rf}) i.e., RCP 2.6, 3.4, 4.5, 6.0 $\mathrm{W/m^2}$. These two parameters are then used to estimate the emission intensity of the electricity generation sector in the future for each of the combinations of SSP and RCP scenarios. The simulated outcome for the SSP2 condition (indicating middle of the road climate action) for various Representative Concentration Pathway (RCP) scenarios is shown in Figure 4. The scenarios are used to represent how decarbonization of energy systems will affect the upstream life-cycles of various alternatives, thereby including future decisions. Mathematically, these emission intensities are surrogated within the planning optimization framework as a piecewise linear function of time, $\mathrm{IAM}_{\tau}=f_3(\mathrm{RCP}_{3.4}, \tau)$ shown in equation 1), ultimately used as a time-dependent correction factor (IAM_{τ}) to the emissions generated from electricity in the selected value-chain solution (Em_k^{elec}).

2.4 Carbon neutrality and Circularity targets as constraints

Since the goal of the proposed framework is to find optimal roadmaps towards meeting future environmental targets, the constraints defined in this section are critical, and are defined by the stakeholders. In certain cases when the targets are for near the end of the time horizon, these targets may represent terminal constraints, however, an additional time-period should be added to extend the time horizon and yield sensible yields for the last time period. The carbon neutrality target can be ensured by adding a constraint such as the following,

$$\begin{aligned} \mathrm{GHG}_{\tau} &= \sum_{k} x_{k,\tau}(\mathrm{Em}_k - \mathrm{Em}_k^{elec}[1 - \mathrm{IAM}_{\tau}]) \quad \forall\, \tau \in \mathbb{T} \\ \mathrm{GHG}_{\tau^*} &\leq 0 \quad \forall\, \tau^* \in \mathbb{T} \text{ s.t. } \overline{\tau}(\tau^*) \geq t^{\mathrm{GHG}=0} \end{aligned} \tag{14}$$

Similarly, recycling/ up-cycling constraints can be imposed on circularity θ, abiding by the Plastics Pact or other organizational constraints to have circularity higher than a threshold (θ^*) for $\overline{\tau}(\tau^*) \geq t^{\theta \geq \theta^*}$. These terminal constraints ensure that the optimal roadmap does satisfy the constraints around Net-zero emissions, carbon neutrality or up-cycling after a user-defined point in the time horizon.

2.5 Carbon budget utilization

While determining the optimal roadmap to meet the emissions target at the end of the time horizon, it is important to ensure that the solution roadmap does not lead to large amounts of greenhouse gas emissions during the time horizon. It is for this reason we formulate a variable tracking the cumulative (or accrued) GHG emissions during the time horizon. As mentioned in the section 2.1, the multi-period planning optimization framework allows for selection of Pareto-optimal solutions to distribute the consumer demand. At each time period, a particular solution can either be selected, deselected or retained. This information is stored in the $y_{k,tt}$ binary variable. Based on the relative importance of carbon budgets in the time horizon, the cumulative GHG emissions objective can either be formulated as a linear approximation or a complex non-linear objective which records the exact time of selection of a solution in a time-period.

In a linear formulation of cumulative greenhouse gas emissions ($\mathrm{GHG}_{\mathrm{cum.}}$), the average emissions from two snapshots of chosen solutions at the beginning and end of any time period ($t = \overline{\tau}_{\tau-1}$ and $t = \overline{\tau}_{\tau}$) are multiplied by the duration of each time period , i.e.,

$(TH)/N$.

$$\mathrm{GHG}_{cum.} = \frac{TH}{2N}\sum_{\tau} \left(\sum_k x_{k\tau-1}\{\mathrm{Em}_k - \mathrm{Em}_k^{elec}[1-\mathrm{IAM}_{\tau-1}]\}\right) + \left(\sum_k x_{k\tau}\{\mathrm{Em}_k - \mathrm{Em}_k^{elec}[1-\mathrm{IAM}_{\tau}]\}\right) \tag{15}$$

The non-linear formulation, on the other hand, would track each transition point over each time period and accurately calculate the net emissions from various value-chain solutions implemented for a non-zero time-span. However, this inclusion in the optimization model would require additional constraints in the multi-period planning formulation to ensure that the functional unit (or consumer demand) has to be met between two separate transitions. This complexity can be avoided by shortening the duration of the time-period without much computational load as the problem scales linearly with increase in number of time periods (N). It can also be avoided through a slightly more complex time-based weighted average of the two emission snapshots. The weights can be estimated as an effective transition point, tt_k, calculated as follows.

$$2(\sum_k \mathbf{1})tt_\tau = \sum_k \left(\sum_k x_{k,\tau-1}\right) t_{k\tau} + \left(\sum_k x_{k,\tau}\right) t_{k\tau} \quad \text{where, } \mathrm{IAM}_\tau = f_3(\mathrm{RCP}_{\mathrm{rf}}, tt_\tau) \tag{16}$$

Correspondingly, the non-linear formulation of cumulative GHG emissions can be formulated as follows.

$$\mathrm{GHG}_{cum.} = \sum_{\tau} tt_\tau \left(\sum_k x_{k\tau-1}\{\mathrm{Em}_k - \mathrm{Em}_k^{elec}[1-\mathrm{IAM}_{\tau-1}]\}\right) + (5-tt_\tau)\left(\sum_k x_{k\tau}\{\mathrm{Em}_k - \mathrm{Em}_k^{elec}[1-\mathrm{IAM}_{\tau}]\}\right) \tag{17}$$

With the weight (tt_k) being a bi-linear function of x_{kt} and t_{kt}, the cumulative GHG emissions becomes a cubic function of the decision variables. Many commercial solvers like Gurobi, can now handle quadratic constraints, therefore the non-linearities in the approximated time-point of shift tt_τ stemming from $t_{k\tau}x_{k\tau}$ in the above equation have been converted to quadratic constraints using McCormick Relaxations.[32] Since, the variables have comparable lower and upper bounds, these affine relaxations are expected to have high convergence and satisfactory tightness.[33] The modified equation for tt_τ which makes the previous equation quadratic is as follows.

$$\begin{aligned} \mathrm{n}(k)tt_\tau &= \sum_{k_1}\left(\sum_{k_2} w^1_{k_1,k_2,\tau}\right) + \left(\sum_{k2} w^2_{k_1,k_2,\tau}\right) \\ \text{where, } {w^1}_{k_1,k_2,\tau} &= \text{McCormick Relaxations}(x_{k_1\tau}, x_{k_2,\tau}, t_{k,\tau}) \\ {w^2}_{k_1,k_2,\tau} &= \text{McCormick Relaxations}(x_{k_1,\tau-1}, x_{k_2,\tau-1}, t_{k,\tau}) \\ &\text{and, } k_1, k_2 \in \mathbb{K} \end{aligned} \tag{18}$$

There are several ways we can penalize large cumulative GHG emissions, including introducing caps (or budgets), taxation, ecosystem capacity caps, etc.[34] In the case study used in this manuscript, we use taxation since it requires a single parameter input, namely carbon tax per kg of CO2 equivalent emission. On the other had estimating carbon budgets and understanding true carrying capacity are still research questions and have considerable subjectivity. In our study, we impose a fixed carbon tax of 120$ per ton CO_2 equivalent emissions emitted during the time horizon[35] and include it within the cost minimization objective.

2.6 Annualized investment cost for eco-innovation adoption

The cost of eco-innovation adoption at a particular time during the time horizon is assumed to be directly proportional to the marginal difference between the expected readiness level ($\mathbb{E}[RL_i](t)$) of the innovation i at time t and the maximum possible value of readiness level (RL_{max}). RL_{max} usually corresponds to the diffusion/ adoption stage. The multiplying factor is a parameter called the marginal cost to increase RL by 1 unit (MCRL). Since, this investment to bring a particular innovation to the diffusion stage happens at a future point in the time horizon, it needs to be discounted for time value of money using a discounting rate of r. Ultimately the cost is incurred only if the innovation is chosen for investment in the time period τ, given by the expression, $(y_{i,\tau+1} - y_{i,\tau})$. The resulting expression for the total investment cost for all chosen innovations is as follows,

$$\text{Investment Cost} = \sum_{\tau\in\mathbb{T}}\sum_{i\in\mathbb{I}}(y_{i,(\tau+1)} - y_{i,\tau})\frac{\text{MCRL}_i[RL_{\max} - \mathbb{E}[RL_i](t_i)]}{(1+r)^{t_i}} \tag{19}$$

As mentioned earlier, inclusion of the detailed stochastic models for RL evolution within optimization is not needed if the decision variables do not affect the transition probabilities or sojourn times of the CTMC. This assumption is valid if climate change models or external investments do not alter the natural evolution profile which may be obtained from historical data. With this assumption, the non-linearity of the expression is eliminated through simulation of CTMCs and creating a piecewise linear surrogate model for each innovation describing the Investment Cost as a function of time ($f_2(t)$). The choice of the continuous decision variable t_i for time of adoption, thus depends on the developed surrogate model. In addition to the investment cost, the cost objective also contains the 'present' value of the operating cost (OPEX) of the chosen compromise solutions on the Pareto front in the time horizon, estimated using the Life-cycle cost of natural resources (LCC) recorded in the input dataset.

3 Case Study

The multi-period planning framework is demonstrated for packaging eco-innovations within the grocery bags value-chain of USA, intended towards net-zero emissions and circularity. These innovations can disrupt any part of the value-chain, which comprises of the cradle-to-cradle network involved in the production, use, re-use, recycling and end-of-life of five types of grocery bags, made from, polyethylene (high and low density), polypropylene, poly-lactic acid and paper. Each kind of bag has a unique volume carrying capacity, weight and re-usability. Innovations can be from any domain including technologies for mechanical or chemical recycling, increasing re-use, segregation programs, etc. A previously developed methodology on screening and ranking eco-innovations identifies 10 most promising alternatives based on a utopia point shift criteria, evaluated using a multi-objective optimization routine on cradle-to-cradle life-cycle networks.[17] The screened innovations are (i) Municipal solid waste (MSW) pyrolysis to olefins, (ii) Source Segregation Programs, (iii) AI-assisted image classification to sort MSW, (iv) Linear alkyl benzenes from waste polyethylene, (v-vii) pyrolysis of segregated plastics, (viii) recycling of poly-lactic acid (PLA) to polymer resin through mononitrile clay catalyst, (ix) alkaline hydrolysis of PLA to lactic acid monomer and (x) alcoholysis of PLA to methyl lactate. The outcome of this methodology is a range of innovative Pareto-fronts, with numerous compromise solutions - choice of which determines the distribution of consumer demand, i.e. annual volume carrying capacity of 100 million households in the USA for grocery shopping. The Pareto-fronts for the 10 chosen innovations for this case-study are presented in figure 3. As described in section 2.1, the optimal roadmap essentially traverses between several Pareto-optimal (or compromise solutions) points in the time dimension, with a Pareto-front becoming available only after a one-time investment. This is achieved using the multi-period formulation described in equation 1.

3.1 Evolution patterns

Technology forecasting of the 10 screened innovations is a critical aspect of the roadmapping framework, as it determines the amount of investment required to make innovative Pareto-optimal solutions adoptable at any particular time using the equation 13. As described in section 2.2.3, this technology forecasting is modeled using stochastic processes, specifically 'Continuous Time Markov Chains'. Due the computational complexity of the analytical solutions of CTMCs, we simulate them before hand for all innovations (or typical categories of these), and surrogate them using piecewise linear functions. Figure 5 depicts the evolution of the 10 screened innovations. As described in section 2.2.3, there are certain practical challenges in obtaining the parameters required to model these CTMCs. Thus, we have relied on insights and values from several industrial stakeholders and collaborators[36] in this work. In the future, limiting behavior will be used to fit CTMC parameters on academic and patent citation data about historic innovations.

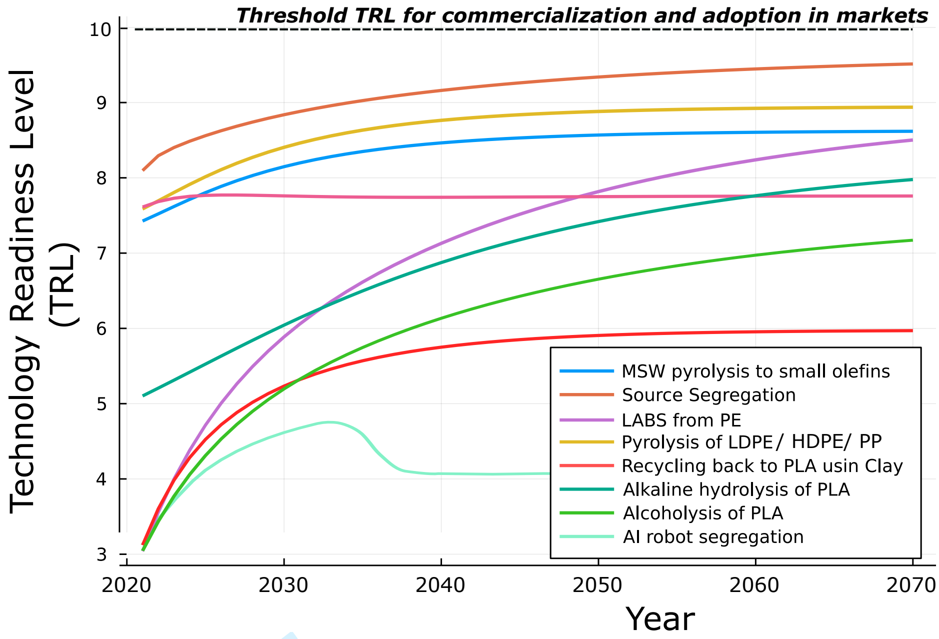


Figure 5: Simulated Continuous Time Markov Chains for the 10 innovations available based on sector they constitute to.

3.2 Climate Change Scenarios

As stated in section 2.3 background decarbonization can drive, inspire and affect future innovations during the long time horizon. In addition to choice of innovation for each climate scenario, the potential of achieving Net-Zero is expected to rely heavily on growing renewable content in electricity grids. Therefore, we have simulated multiple profiles of expected emission intensity across the time horizon. This is calculated using the projected emissions from electricity sector divided by the expected demand of electricity at any time, for different Representative Concentration Pathways under the Middle of the road shared socio-economic pathway (SSP2). The resulting emission intensity profiles are shown in figure 4, and are used to update the upstream scope 2 emissions from electricity for grocery-bags production and end-of-life treatment as described in section 2.3.

3.3 Results and Discussions

The multi-period planning model is implemented under several constraints and projections for reaching the targets set for the grocery bags value-chain. The targets are mainly the following,

- Net-Zero GHG Emissions by 2050, computed for a life-cycle system boundary.
- Up-cycling, 2035 onwards; indicated by the value of monetary circularity exceeding 1 ($\theta \geq 1$). θ is defined as the ratio of monetary value restored through circular flows to the manufacturing cost.

While most of the aspects of the case study are real and can be introduced with high confidence, some are educated guesses for the prototype, particularly R&D Marginal cost per RL increase (MCRL), CTMC parameters, carbon tax rate, etc. For instance, the MCRL has been arbitrarily set to 10 million USD per RL increase. This is done due to lack of data, and is kept identical for all innovations to prevent it from biasing the solution. In addition, modeling of CTMCs for several innovations relies on subjective inputs from industrial stakeholders, and currently lack quantitative basis. Cost of Carbon Dioxide emissions in the future is assumed to be a static 120$ per ton, which will most likely not be the case and will evolve across the time horizon. Future work intends to address these practical challenges in obtaining results with higher confidence using uncertainty quantification, robust optimization, fitting CTMC parameters using historic data and finally appropriate slab-wise carbon costing models. The results presented in this manuscript, must therefore be viewed more as an application of the framework with special attention to its ability to provide optimal roadmaps with numerous considerations, instead of identifying the exact solutions and promising innovations for the grocery bags case study.

The outcome of implementing the roadmap optimization framework is a gantt chart denoting the adoption of various Innovative Pareto-optimal value-chain solutions at different points of time. For RCP 3.4 under the SSP2 scenario, the optimal gantt chart (or roadmap) is shown in Figure 6. The corresponding GHG emissions, circularity and operating cost profiles across the time horizon are shown in figure 7. It can be seen from these results that Pyrolysis of sorted LDPE using FCC catalyst is chosen for immediate investment, as it would reduce the exploitation of carbon budgets at the lowest expense. Next, linear alkyl benzenes is chosen starting 2035, after which it gets to a high enough TRL and is lucrative to ensure that the up-cycling requirements are being met. Ulti-

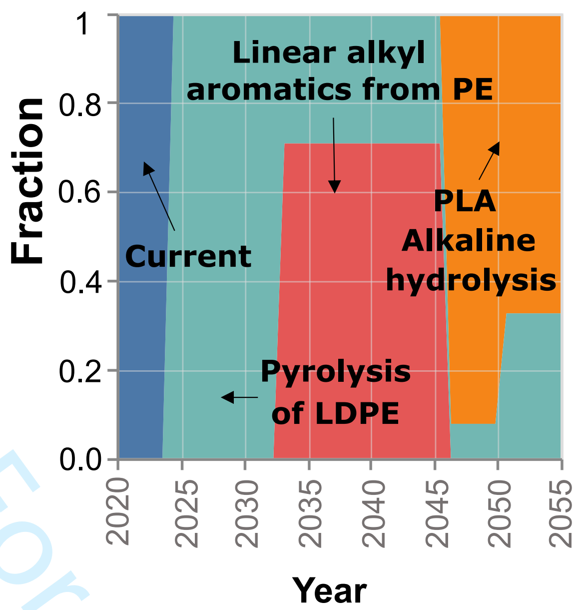


Figure 6: Result for SSP2 RCP 3.4 Scenario: Optimal combination of innovations selected during the time horizons to meet GHG Emissions and Circularity targets while minimizing investment costs, value-chain operating costs and carbon taxes.

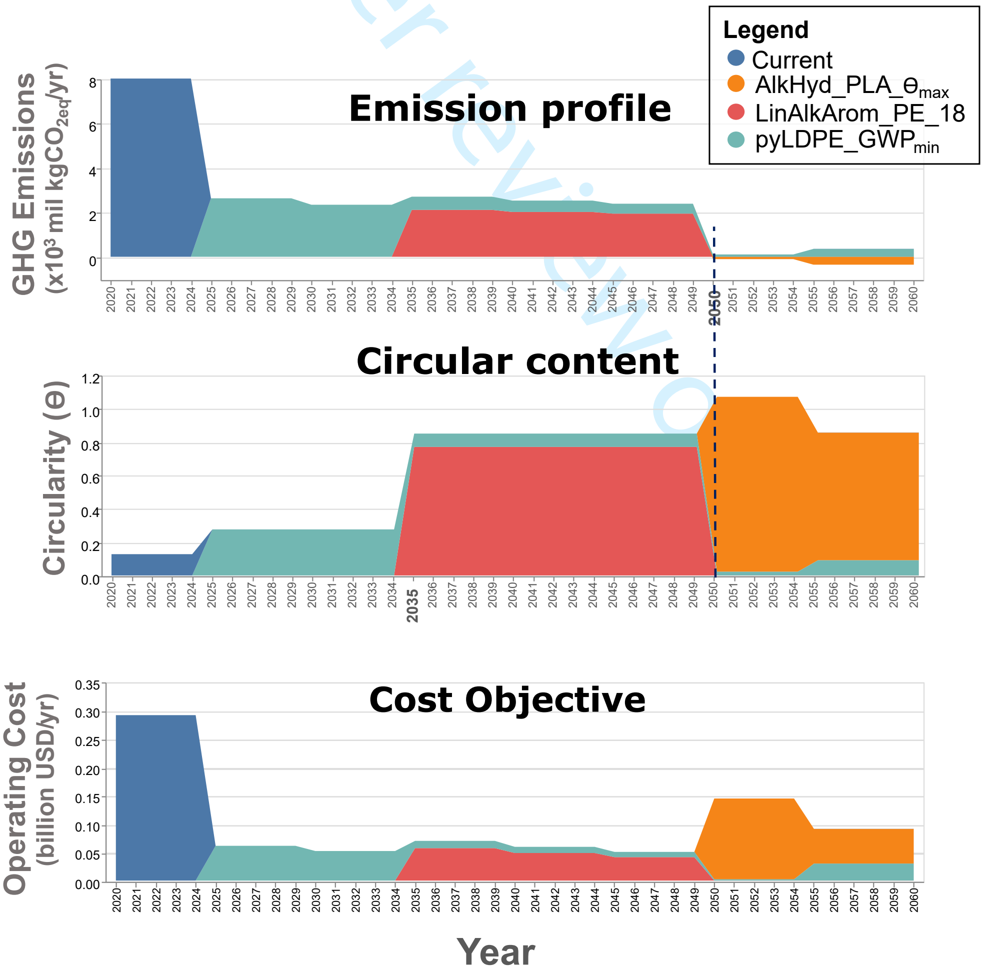


Figure 7: Result for SSP2 RCP 3.4 Scenario: GHG Emissions, Circularity and Operating cost (or Resource-use cost) profiles as a function of time for the optimal roadmap.

mately, bio-based PLA bags start getting selected starting 2050, as they contribute to emission reduction through displacing conventional lactic acid through alkaline hydrolysis and biogenic carbon sequestration. Despite an initial low TRL, this innovation is expected to have an upward evolution (according to CTMCs in figure 5). This, along with time value of money being lower in the future, encourages a late investment and shift to bio-based PLA alternatives. As seen from figure 7, Life-cycle GHG emissions become net-zero starting 2050 and circularity targets are being met by 2035. Evidently, this roadmap takes into account several phenomena including technology evolution, climate change policy, annualized operating and R&D costs, as stated in section 2, thereby providing a holistic roadmap towards meeting environmental targets at lowest cost.

Multiple climate change and projected policy changes of the future are constructed as scenarios using IAM models. Roadmaps corresponding to these scenarios are shown in figure 8a. Evidently, net-zero GHG emissions are possible only for some of the scenarios with more stringent climate action policy that ensure a Representative Concentration Pathway (RCP) of at most 3.4 W/m^2. Notably, even an intermediate scenario of RCP 4.5 W/m^2 will be able to mitigate only 91% of emissions from the grocery bags value-chain by 2050. This means that it will not be possible for grocery bags to meet a net-zero emission goal due to high scope 2 and scope 3 emissions from upstream life-cycle processes. In addition to this insight, the innovations robust to climate change policy are also found on the basis of their selection for over 3 RCP radiative forcing scenarios, to be the following.

- Pyrolysis of LDPE using FCC-based catalyst
- Alkaline Hydrolysis of PLA to lactic acid
- Bio-based polyethylene at scale

This framework can therefore be used by companies and organizations to not only plan their sustainability transitions to Net-zero at lowest cost, but also identify investment alternatives which would help them be robust to future climate action policy. It is worthwhile to note that with worsening future scenarios, the cost objective also deteriorates due to requirements of more expensive investments and higher carbon budget utiliza-

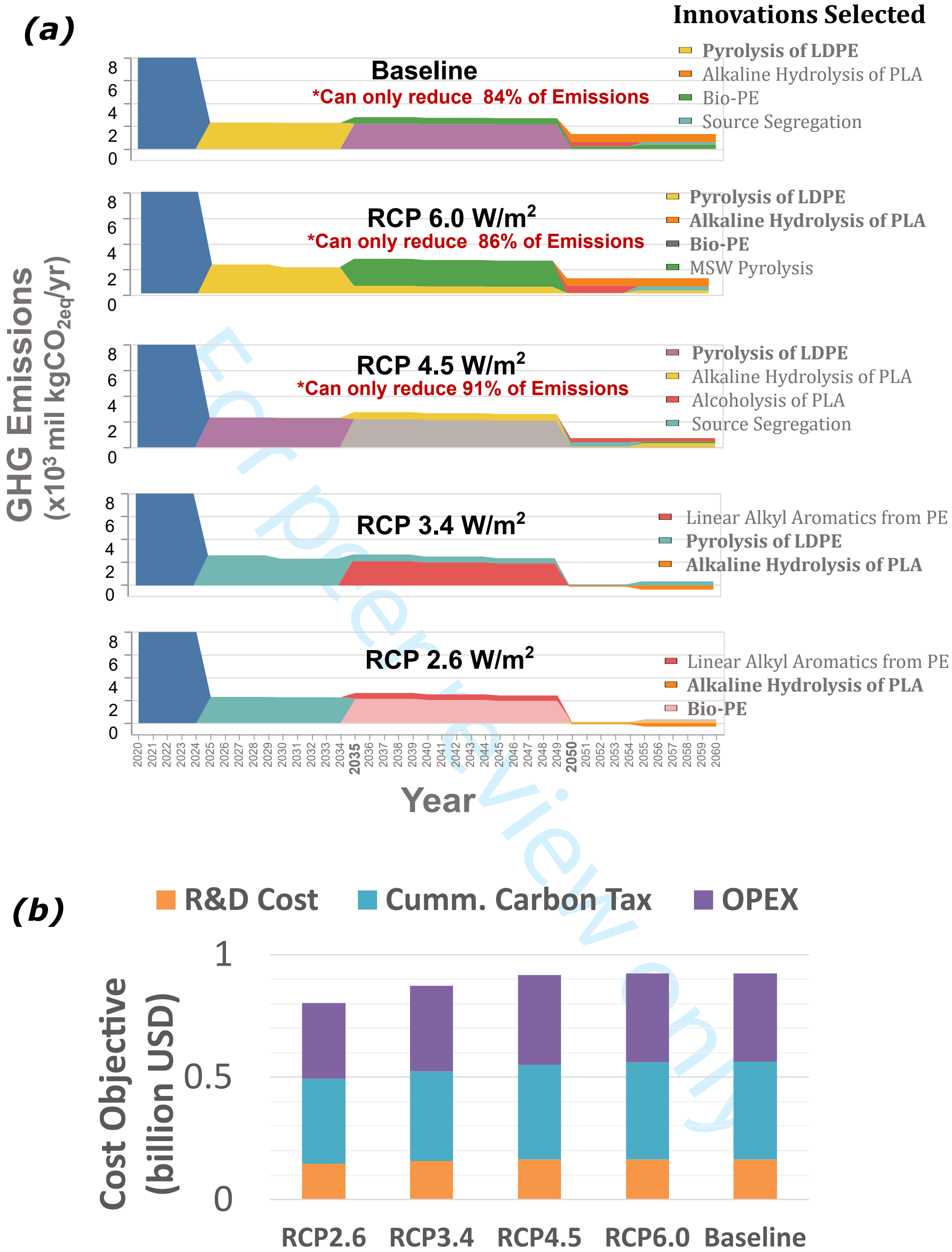


Figure 8: (a) GHG Emissions profiles for optimal roadmaps under several climate change scenarios (RCP 2.6, 3.4, 4.5, 6.0 and Baseline) under the socio-economic pathway SSP2. Net-zero GHG emissions from the grocery bags value-chains is not possible for scenarios worse than RCP 3.4 W/m^2. Innovations robust to climate change effects and policy are also found (bold-faced). (b) Worse climate change scenarios correspond to higher investment costs and carbon taxes, owed by the grocery bags value-chain and the packaging industry.

tion (or taxation), as shown in figure 8b. This implies that an optimal roadmap to a carbon-neutral sustainable circular economy would favor the industry (especially plastic packaging) to promote and back sustainability-related climate action policy for the entire supply chain.

4 Conclusions

The developed multi-period planning framework is capable of designing optimal roadmaps towards meeting corporate or national environmental targets around greenhouse gas emissions and circularity, at minimal investment and operating costs. It also considers effects of changing climate action policy and evolving technology readiness levels based on stochastic models. The framework is general and applicable to any product system or supply chain with input data in the form of either innovative Pareto-fronts developed using previous work[17,20] or set of alternative value-chain alternatives corresponding to each innovation. The outcomes of the framework include (a) minimal cost roadmap to meet targets, (b) investment strategy with what and when decisions, (c) potential of achieving environmental targets given the background scenarios of climate change, and (d) innovations which are robust to climate action policy. In this manuscript, the framework has been applied for guiding sustainability transitions to the grocery bags value-chain network with innovations from the packaging technology, social behavior, feedstock manufacturing and several other domains. Ultimately, out of the 10 screened eco-innovations targeted towards sustainable circular economy of grocery bags value-chain, optimal roadmap is likely to choose the three alternatives to meet targets, namely advanced Pyrolysis of low-density polyethylene waste to fuel, alkaline hydrolysis of polylactic acid to lactic acid, and bio-based bio-polyethylene. These innovations are found to be robust to multiple possible scenarios of climate change and corresponding policy. These also ensure minimal utilization of carbon budgets through reduction in cumulative GHG emissions. As demonstrated using the case study, the developed framework can be very useful to industry and policy-makers to guide future transitions towards Net-zero greenhouse gas emissions and circularity - while considering holistic life-cycle system boundaries, future climate change scenarios and forecasts of technology evolution. In the future, models for technology forecasting will be validated for clusters of similar technologies using historical data. In addition, a detailed sensitivity analysis will be conducted to probe the effects of parameters such as carbon tax (in USD per ton), R&D costs and discounting rates on the optimal roadmap selection.

Acknowledgments

Funding for this work was provided by the Michael and Gretchen Mavrovouniotis Philanthropic Foundation, Global Kaiteki Center at Arizona State University, the National Science Foundation through grant EFMA-2029397 and the Richard M. Morrow professorship fund.

Data Availability

The supporting information contains a document guide to access the data and code (attached zip folder) to utilize the framework either for a user defined dataset, or to reproduce the results from this case study. The datasets and code have also been provided in a GitHub repository[37] as Jupyter notebooks with appropriate markdowns and package requirements.

References

[1] Simon L Lewis and Mark A Maslin. Defining the anthropocene. *Nature*, 519(7542):171–180, 2015.

[2] Johan Rockström, Will Steffen, Kevin Noone, Åsa Persson, F Stuart Chapin III, Eric Lambin, Timothy M Lenton, Marten Scheffer, Carl Folke, Hans Joachim Schellnhuber, et al. Planetary boundaries: exploring the safe operating space for humanity. *Ecology and society*, 14(2), 2009.

[3] Andrea Valencia, Wei Zhang, and Ni-Bin Chang. Sustainability transitions of urban food-energy-water-waste infrastructure: A living laboratory approach for circular economy. *Resources, Conservation and Recycling*, 177:105991, 2022.

[4] Bruno Turnheim, Mike Asquith, and Frank W Geels. Making sustainability transitions research policy-relevant: Challenges at the science-policy interface. *Environmental innovation and societal transitions*, 34:116–120, 2020.

[5] Ana Maria Vicedo-Cabrera, Yuming Guo, Francesco Sera, Veronika Huber, Carl-Friedrich Schleussner, Dann Mitchell, Shilu Tong, Micheline de Sousa Zanotti Stagliorio Coelho, Paulo Hilario Nascimento Saldiva, Eric Lavigne, et al. Temperature-related mortality impacts under and beyond paris agreement climate change scenarios. *Climatic change*, 150:391–402, 2018.

[6] Energy & Climate Intelligence Unit, Data-driven EnviroLab, and NewClimate Institute. Net zero tracker companies, 2022. Accessed on 13th May, 2023.

[7] Chandni Singh, Soundarya Iyer, Mark G New, Roger Few, Bhavana Kuchimanchi, Alcade C Segnon, and Daniel Morchain. Interrogating effectiveness in climate change adaptation: 11 guiding principles for adaptation research and practice. *Climate and Development*, 14(7):650–664, 2022.

[8] Glenn A Aguilar-Hernandez, Carlos Pablo Sigüenza-Sanchez, Franco Donati, Stefano Merciai, Jannick Schmidt, João FD Rodrigues, and Arnold Tukker. The circularity gap

of nations: A multiregional analysis of waste generation, recovery, and stock depletion in 2011. *Resources, Conservation and Recycling*, 151:104452, 2019.

[9] Jannik Giesekam, Jonathan Norman, Alice Garvey, and Sam Betts-Davies. Science-based targets: on target? *Sustainability*, 13(4):1657, 2021.

[10] Jonathan Köhler, Frank W Geels, Florian Kern, Jochen Markard, Elsie Onsongo, Anna Wieczorek, Floortje Alkemade, Flor Avelino, Anna Bergek, Frank Boons, et al. An agenda for sustainability transitions research: State of the art and future directions. *Environmental innovation and societal transitions*, 31:1–32, 2019.

[11] Haijian Si, Stylianos Kavadias, and Christoph Loch. Managing innovation portfolios: From project selection to portfolio design. *Production and Operations Management*, 2022.

[12] N Loukeris, D Donelly, A Khuman, and Y Peng. A numerical evaluation of meta-heuristic techniques in portfolio optimisation. *Operational Research*, 9(1):81–103, 2009.

[13] Marian Beise and Klaus Rennings. Lead markets and regulation: a framework for analyzing the international diffusion of environmental innovations. *Ecological economics*, 52(1):5–17, 2005.

[14] Coen van der Giesen, Stefano Cucurachi, Jeroen Guinée, Gert Jan Kramer, and Arnold Tukker. A critical view on the current application of lca for new technologies and recommendations for improved practice. *Journal of Cleaner Production*, 259:120904, 2020.

[15] Stefan Pauliuk, Anders Arvesen, Konstantin Stadler, and Edgar G Hertwich. Industrial ecology in integrated assessment models. *Nature Climate Change*, 7(1):13–20, 2017.

[16] Vyom Thakker and Bhavik R Bakshi. Designing value chains of plastic and paper carrier bags for a sustainable and circular economy. *ACS Sustainable Chemistry & Engineering*, 9(49):16687–16698, 2021.

[17] Vyom Thakker and Bhavik R Bakshi. Ranking eco-innovations to enable a sustainable circular economy with net-zero emissions. *ACS Sustainable Chemistry & Engineering*, 2023.

[18] Manuel Díaz-Madroñero, David Peidro, and Josefa Mula. A review of tactical optimization models for integrated production and transport routing planning decisions. *Computers & Industrial Engineering*, 88:518–535, 2015.

[19] Manuel Díaz-Madroñero, Josefa Mula, and David Peidro. A review of discrete-time optimization models for tactical production planning. *International Journal of Production Research*, 52(17):5171–5205, 2014.

[20] Vyom Thakker and Bhavik R. Bakshi. Toward sustainable circular economies: A computational framework for assessment and design. *Journal of Cleaner Production*, page 126353, 2021.

[21] Vyom Thakker and Bhavik R Bakshi. Multi-scale sustainable engineering: Integrated design of reaction networks, life cycles, and economic sectors. *Computers & Chemical Engineering*, 156:107578, 2022.

[22] Mark AJ Huijbregts, Zoran JN Steinmann, Pieter MF Elshout, Gea Stam, Francesca Verones, Marisa Vieira, Michiel Zijp, Anne Hollander, and Rosalie Van Zelm. Recipe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level. *The International Journal of Life Cycle Assessment*, 22:138–147, 2017.

[23] Vyom Thakker and Bhavik R Bakshi. Guiding innovations and value-chain improvements using life-cycle design for sustainable circular economy. In *Computer Aided Chemical Engineering*, volume 49, pages 1945–1950. Elsevier, 2022.

[24] Marvin B Lieberman. The learning curve, diffusion, and competitive strategy. *Strategic management journal*, 8(5):441–452, 1987.

[25] Edward S Rubin, Sonia Yeh, Matt Antes, Michael Berkenpas, and John Davison. Use of experience curves to estimate the future cost of power plants with co2 capture. *International journal of greenhouse gas control*, 1(2):188–197, 2007.

[26] Robert J Dolan and Abel P Jeuland. Experience curves and dynamic demand models: Implications for optimal pricing strategies. *Journal of Marketing*, 45(1):52–62, 1981.

[27] Melissa A Schilling and Melissa Esmundo. Technology s-curves in renewable energy alternatives: Analysis and implications for industry and government. *Energy policy*, 37(5):1767–1781, 2009.

[28] Google LLC and AFARA. Closing the circularity gap, link: https://www.gstatic.com/gumdrop/sustainability/closing-plastics-gap-full-report.pdf, accessed on: 7th september, 2022. Technical report, 2022.

[29] Everett M Rogers. Diffusion of preventive innovations. *Addictive behaviors*, 27(6):989–993, 2002.

[30] Tom Lee and Louis L Wilde. Market structure and innovation: A reformulation. *The Quarterly Journal of Economics*, 94(2):429–436, 1980.

[31] Angelica Mendoza Beltran, Brian Cox, Chris Mutel, Detlef P van Vuuren, David Font Vivanco, Sebastiaan Deetman, Oreane Y Edelenbosch, Jeroen Guinée, and Arnold Tukker. When the background matters: using scenarios from integrated assessment models in prospective life cycle assessment. *Journal of Industrial Ecology*, 24(1):64–79, 2020.

[32] Angelos Tsoukalas and Alexander Mitsos. Multivariate mccormick relaxations. *Journal of Global Optimization*, 59(2):633–662, 2014.

[33] Jaromił Najman and Alexander Mitsos. On tightness and anchoring of mccormick and other relaxations. *Journal of Global Optimization*, 74:677–703, 2019.

[34] Jeremy Carl and David Fedor. Tracking global carbon revenues: A survey of carbon taxes versus cap-and-trade in the real world. *Energy Policy*, 96:50–77, 2016.

[35] Yves Steinebach, Xavier Fernández-i Marín, and Christian Aschenbrenner. Who puts a price on carbon, why and how? a global empirical analysis of carbon pricing policies. *Climate Policy*, 21(3):277–289, 2021.

[36] Fatima Hafsa, Kevin J Dooley, George Basile, and Rajesh Buch. A typology and assessment of innovations for circular plastic packaging. *Journal of Cleaner Production*, 369:133313, 2022.

[37] Vyom Thakker and Bhavik R Bakshi. Mapping the path to a carbon neutral circular economy by long-term planning with changes in technologies, energy mix, and climate - code repository, https://github.com/vyom-thakker/RoadmapsIAM/tree/manuscript. Technical report, 2023.