Assessing the Environmental and Societal Impacts of Carbon Capture, Utilization, and Storage (CCUS) Technologies and Products

by

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Abstract

Annual atmospheric levels of carbon dioxide (CO_2) have risen from 11 Gt in 1960s to 36.6 Gt in 2023. In order to mitigate the global warming impact, the implementation of carbon capture, utilization, and storage technologies (e.g., negative emission technologies (NETs)) is crucial to prevent rising carbon emissions and achieve climate stabilization. NETs encompass various strategies including carbon capture and storage with bioenergy, direct air capture, enhanced weathering, reforestation, afforestation, oceanic sequestration, agricultural practices, and biochar. Recent advancements also have introduced novel carbon removal approaches, such as chemical looping combustion for CO_2 capture, the use of CO_2 in beverage carbonation, and its storage in basalt and ultramafic rocks through carbon mineralization. However, the environmental and human health implications associated with the social perspective of increasingly emerging CCUS technologies and carbon-negative products have yet to be thoroughly analyzed. Therefore,

employing systems thinking and a holistic approach to evaluate the sustainability performance of these technologies and products is essential for informed decision-making.

One way to estimate environmental impacts is by utilizing the life cycle assessment (LCA) methodology. The first LCA (chapter 2) study highlighted significant research gaps through a literature review on enhanced weathering for carbon sequestration, specifically focusing on wollastonite. It found that natural wollastonite is preferable for carbon capture due to its lower environmental and health impacts compared to synthetic forms, which showed a dramatic increase in these impacts when transitioning from natural sources; however, increasing production efficiency from 60% to 99% could potentially reduce environmental impacts by 55%68%. The second LCA study (Chapter 3) assessed the environmental and health impacts of producing 1 gram of polyhydroxybutyrate (PHB) via electrochemical and biosynthesis processes, identifying the electrochemical process as the major contributor to these impacts. This study emphasized that the choice of raw materials, the production technologies used, the duration of the experiment, and the efficiency of the output significantly influence the overall environmental and health outcomes.

A social perspective on the adoption of CO_2-based single-use bioplastic bottles was offered. The third paper (Chapter 4), through surveys, reveals a strong U.S. consumer interest in sustainable materials, with positive attitudes and a willingness to pay a premium for CO_2-based bioplastics. These findings highlight a substantial demand for sustainable product options and provide valuable insights for marketing strategies. The fourth paper (Chapter 5) utilizes Agent-Based Modeling (ABM) to model the factors influencing the adoption of these bioplastic bottles, emphasizing that lower costs and reduced environmental footprints enhance adoption rates, while higher costs and greater environmental impacts stop it. The study also indicated the importance of social dynamics, showing that strong strength of the social network can significantly promote adoption, especially in closed communities, and highlights the need for strategies that balance economic feasibility and environmental benefits.

Collectively, the LCA reveals that the carbon-negative technologies or products are not truly carbon-negative due to the positive carbon emissions generated during manufacturing processes. Additionally, the consumer surveys and ABM demonstrated a strong demand for sustainable CO_2-based bioplastics that are influenced by cost, environmental impact, and social dynamics, underscoring the importance of balanced strategies for promoting adoption. Despite recent advancements in CCUS and carbon-negative products, a thorough analysis of their environmental and human health implications from a social perspective is still needed. This emphasizes the importance of a holistic approach and systems thinking in sustainability assessments.

Dedication

I would like to dedicate this work to my parents. Thank you for your support. Also, I would like to dedicate this dissertation to the memory of my grandparents. I love you all.

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Table of Contents

List of Figures

Lists of Tables

1. Introduction

1.1. Research Summary and Goals

When viewed from a non-expert perspective, carbon capture, utilization, and storage (CCUS) technologies might seem to have numerous advantages in the fight against climate change, capturing carbon dioxide (CO_2) directly from industrial sources or even from the atmosphere. The premise is straightforward reducing the carbon footprint of Anthropocene by capturing greenhouse gases before or after they are released into the atmosphere. This could lead one to assume that CCUS has minimal impact on environmental degradation or resource depletion, such as the consumption of water and energy supplies. However, a deeper scientific analysis reveals a more complex picture. While CCUS holds significant promise for reducing atmospheric CO_2 levels and mitigating climate change, the technology itself is energy-intensive, involves substantial material inputs, and poses logistical and economic challenges. As the demand for sustainable and effective climate solutions grows, understanding the full lifecycle impacts and improving the efficiency of CCUS technologies become imperative. This is especially critical as these technologies begin to scale up and integrate into various industrial processes worldwide.

Consumer adoption of CCUS technologies can be further enhanced by transparent communication regarding the tangible environmental and economic benefits they offer, such as potential energy savings and subsidies for adopting green technologies. Additionally, building trust through demonstrated successes and reliability in pilot projects can motivate consumers to support and participate in the scaling up of CCUS solutions, recognizing their crucial role in mitigating climate change impacts.

The aim of this research is to investigate the environmental impacts of CCUS technologies and consumer acceptance of CCUS products. Life cycle assessment (LCA) and Agent-based modeling (ABM) were used to analyze the environmental benefits and consumer behavior.

1.2. Research questions and objectives

Existing literature estimates the environmental implications of various CCUS technologies and CCU products with varying scopes, and system boundaries as well as environmental categories.

These considerations shaped the framework of this research and resulted in the research questions:

Question 1: What are the environmental implications of enhanced weathering for CCS using natural and synthesized wollastonite? What are the carbon payback period/breakeven points of these two scenarios? (Chapter 2)

Question 2: What are the environmental implications of bioplastic (polyhydroxybutyrate (PHB)) production using captured CO_2 as feedstock (CCU) via electrochemical and biosynthesis processes? Does PHB have lower environmental and human health impacts compared to petroleum (polyethylene terephthalate (PET)) production? Should PHB substitute conventional plastic to be widely used in the market? (Chapter 3)

Question 3: Are consumers willing to buy CCU products, utilizing an example case study of single-use plastic bottles? How much are they willing to pay for the new products compared to the PET single-use water bottles? (Chapter 4)

Question 4: How do consumers adopt CCU products, especially single-use bioplastic water bottles? Which factors have the most impact on their decision? (Chapter 5)

To address the research gaps and generate new insights into CCUS technologies and products, the following objectives are set up in order to accomplish the aims of this project:

Objective 1: Estimate and compare the environmental implications and CO_2 payback of enhanced weathering for carbon capture and storage (CCS) using wollastonite rock. (Chapter 2)

Objective 2: Analyze the environmental and human health implications of bioplastic production using CO_2 as feedstock via electrochemical and bio-synthesis processes using primary data. (Chapter 3)

Objective 3: Develop a survey to understand the purchase behavior for CO_2 captured bioplastic bottles and the awareness of climate change. The survey will gain valuable insight into the bioplastic bottles replace conventional plastic bottles. (Chapter 4)

Objective 4: Develop an Agent-based model to understand the consumer adoption of CO_2-based bioplastic bottles. (Chapter 5)

1.3. Life cycle assessment (LCA)

A tool called life cycle assessment (LCA) is used to evaluate the environmental and human health impacts of a system or product over the course of either its entire or a portion of the life cycle. Tradeoffs throughout life cycle stages are able to be accounted via LCA. The boundaries of LCA are established based on the goal and scope of the question to be answered by the analysis. These can range from cradle-to-grave, gate-to-grave, cradle-to-gate, or even from cradle-to-cradle. Depending on the question considered the LCA may or may not include transportation. According to ISO 14040, some components of an LCA must be included while others are optional and up to the practitioner's judgment (ISO, 2006a).

The International Standards Organization (ISO) has standardized LCA technique through ISO 14040 (ISO, 2006a) and ISO 14044 (ISO, 2006b). While the ISO 14044 describes the prerequisites and best practices for carrying out an LCA, the ISO 14040 describes the LCA's guiding principles and frameworks. Figure 1 shows the definition of the purpose and scope, inventory analysis, impact assessment, and interpretation. The databases Ecoinvent (Wernet et al., 2016) and U.S. Life Cycle Inventory Databases (USLCI) (National Renewable Energy Laboratory, 2012) will be used along with the SimaPro 9.2.0 software (PRé Sustainability, 2021).

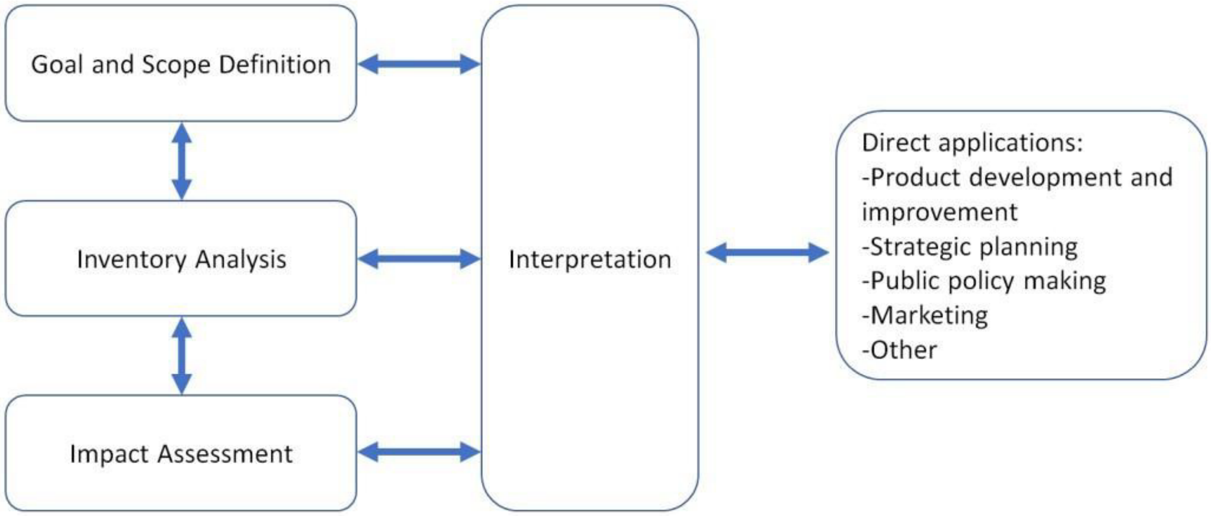

Figure 1. Stages of an LCA (adapted from ISO 14040) (ISO, 2006a).

1.3.1. Goal and scope definition

As described by ISO 14040, declaring the goal of project is the first step of an LCA. Before starting analysis, the functional unit(s) and the scenario(s) should be determined, and system boundaries should also be established in order to suit the goals and scope of the question to be answered by the analysis. The functional unit is a significant component of a LCA study, which is defined as the "quantified performance of a product system for use as a reference unit" by ISO 14040 (ISO, 2006a). Additionally, the system boundary is crucial to determine the whole life stages of a product or service for effective decision making. Four life cycle stages of a product or service are defined, including raw material extraction, manufacturing, use, and end-of-life. These four stages can be taken into account in various combinations, such as cradle-to-gate (raw material extraction and manufacturing stages), cradle-to-grave (all four stages), and cradle-tocradle (all four stages and recycling materials at the end-of-life). The cradle-to-grave system boundary is required for a holistic LCA, but the selection should depend on the scope of the project (Simonen, 2014).

1.3.2. Inventory analysis

In this step, the life cycle inventory (LCI) data is collected from literature, industry, or experimentally. The quantitative data about the inputs of materials, transportations, and energy, as well as the outputs of waste and emissions were collected within the defined system boundaries. Figure 2 presented the inventory data framework for a unit process based on different system boundaries.

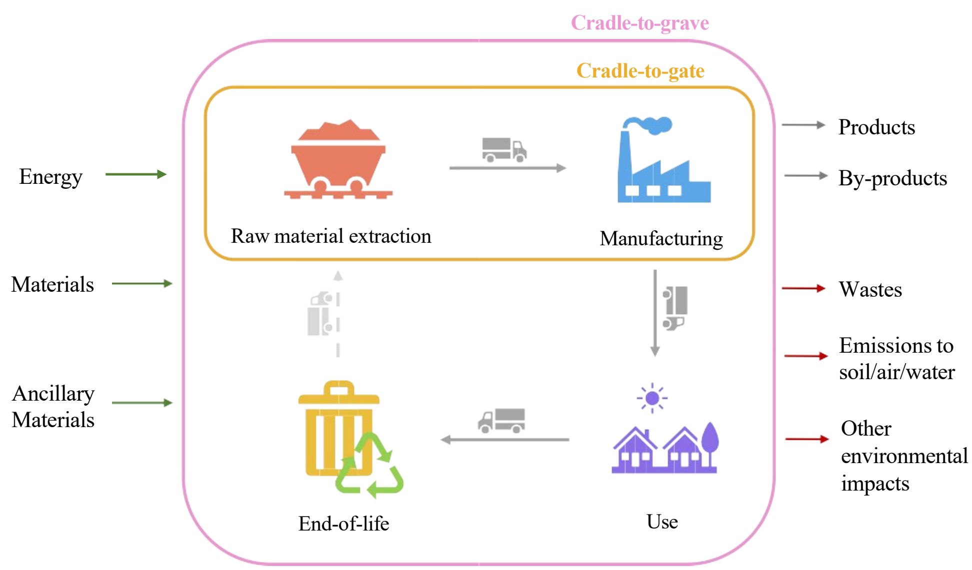

Figure 2. The system boundary of different life cycle frameworks.

1.3.3. Life cycle impact assessment (LCIA)

According to ISO 14040, the selection of impact categories, category indicators, and characterization models, assignment of LCI results, and estimation of category indicator results are all required components of the LCIA phase. The LCIA phase's optional components include normalization, grouping, and weighting. The mandatory requirements for our proposal in the LCIA phase must be met, while the optional elements will not be considered. The Tool for the Reduction and Assessment of Chemical and other Environmental Impacts (TRACI) is an example for environmental and human health implications estimation. The TRACI method is a midpoint approach which is developed by U.S. EPA and based on comprehensive and accountable data and models available in the U.S. (Ghamkhar et al., 2022a). The impact categories include seven environmental indicators (ozone depletion (OD, kg CFC-11 eq), global warming potential (GWP, kg CO_2 eq), smog (SM, kg O_3 eq), acidification (AC, kg SO_2 eq), eutrophication (EU, kg N eq), ecotoxicity (ET, CTUe), and fossil fuel depletion (FFD, MJ surplus)), and three human health indicators (carcinogenic (HHc, CTUh), non-carcinogenic (HHnc, CTUh), and respiratory effects (RE, kg PM2.5 eq)).

Another common method example for LCIA is ReCiPe. The ReCiPe method was developed by for analysis in Europe and includes both midpoint (environmental and human health implication indicators) and endpoint (human health/ecosystem damage indicators) approaches (Rashedi and Khanam, 2020). The environmental and human health impacts indicators are climate change, ozone depletion, terrestrial acidification, freshwater eutrophication, marine eutrophication, human toxicity, photochemical oxidant formation, particulate matter formation, terrestrial ecotoxicity, freshwater ecotoxicity, marine ecotoxicity, ionising radiation, agricultural land occupation, urban land occupation, natural land transformation, water depletion, metal depletion and fossil depletion. Three endpoint indicators are human health, ecosystems and cost increases in resource extraction.

TRACI method is used in this research for implication analysis as all research projects are located in U.S., and it provides multiple impact categories from which potential tradeoffs can be explored.

1.3.4. Interpretation

In accordance with ISO 14040, interpretation comes last in the LCA process. According to the ISO 14044, interpretation entails three steps: identifying significant issues based on the outcomes of the LCI and LCIA phase, evaluating the results for completeness, consistency, and sensitivity, and finally making conclusions, limitations, and providing recommendations related to the goal and scope definition (ISO, 2006b). These approaches are used to appraise the LCA data for completeness, determine the analysis's responsiveness to various input sources, and examine the overall study to ensure the analysis's internal consistent (Simonen, 2014). Given the uncertainties associated with emerging technologies, the use of these methods is essential in the context of this dissertation.

1.4. Agent-based modeling (ABM)

LCA employs a functional unit that accurately reflects the intended purpose and usage of a product or service, allowing for both product/service comparisons and hotspot analysis to identify areas for environmental improvement to minimize the environmental footprint. Nevertheless, LCA faces challenges in modeling human behavior and real-world scenarios, often requiring simplification through idealized assumptions (Morris and Hicks, 2022a). In contrast, Agent-Based Modeling (ABM) has shown promise in overcoming these limitations (Koide et al., 2023). ABM is a computational modeling technique used to simulate the behavior and interactions of individual agents or entities, offering a valuable means to explore complex systems where individual behaviors influence collective outcomes, while LCA remains more common in environmental analysis (Hicks, 2022), ABM's potential in addressing challenges related to human behavior and real-world scenarios is increasingly recognized.

ABM is a valuable tool for complementing LCA and advancing the field of industrial ecology (IE). It helps address questions that LCA alone may not fully answer. ABM has a track record of systematically analyzing various industries and processes, such as simulating energy markets and greenhouse gas emissions (Batten, 2009), urban development (Baynes, 2009), tracking the flow of metal demand (Bollinger et al., 2012), modeling energy infrastructure (Davis et al., 2009), understanding air transport networks (Keirstead and Sivakumar, 2012), and crop modeling (Miller et al., 2013). Another big part of ABM is ABM offers the unique capability to explore various policy scenarios, allowing researchers to investigate the potential impact of interventions such as subsidies on bioplastic bottles, etc.

This work models the potential impact of the adoption of CO_2-based bioplastic bottles and the willingness to purchase this product using an ABM approach. A linear utility function is employed to evaluate the benefits, where each agent evaluates the utility of plastic bottle types ($U_{\text{plastic bottle}}$) based on the characteristics of factors (C_1 through C_n) of the option weighted by the importance of each factor to the agent when selecting plastic bottle types (W_1 through W_n):

$$U_{plastic\ bottle} = C_1W_1 + C_2W_2 + \cdots + C_nW_n \quad \text{Equation 1}$$

where, *C* represents the physical characteristics (e.g., cost, durability, environmental footprint, etc.); *W* represents the weighting data which is informed by survey data.

The utility is used to define the probability of the agent adopting the particular bioplastic bottle technology:

$$P_T = 1 = \sum_{i=1} P_i = \frac{U_i}{U_{bio} + U_{conv}} \quad \text{Equation 2}$$

where P_i is the probability of water bottle i selected, based on the utility of water bottle i, utility of bioplastic water bottle (U_{bio}), and utility of conventional plastic water bottle (U_{conv}) to that particular agent. The probabilities of selection of the two kinds of water bottle sum to 1, meaning the probability of one of the water bottles being selected is certain.

1.5. Details related to each chapter

1.5.1. Chapter 2

Carbon dioxide (CO_2) has been released into the atmosphere continuously due to the consumption of fossil fuels since the Industrial Revolution. The annual global carbon emissions significantly increased from 8.9 Gt CO_2 in 1959 to 36.1 Gt CO_2 in 2022 (Li et al., 2024).

Enhanced weathering (EW) is one of the negative emission technologies (NETs) to remove carbon dioxide (CO_2) and stabilize climate in the future. The definition of EW is using silicate rocks to react with the CO_2 from the air to produce the dissolved products, and then often transporting and storing the final products in the deep layer in the ocean permanently. The most common silicate rocks are basalt and olivine. However, no one has considered wollastonite as the raw material for EW. There are several advantages to using wollastonite rather than basalt and olivine. First, wollastonite reacts more quickly with CO_2 compared to minerals like basalt and olivine due to its higher dissolution rate (Sanna et al., 2014). This rapid reaction facilitates the faster formation of calcium carbonate ($CaCO_3$), a stable and environmentally benign carbonate mineral. This aspect of wollastonite is beneficial for CO_2 sequestration projects where quick reaction times are crucial. Additionally, the process of converting wollastonite into calcium carbonate is less energy-intensive compared to olivine and basalt (Lackner et al., 1995a). This is due to the more favorable thermodynamics of the wollastonite reaction, which can occur at lower temperatures and pressures (Gadikota et al., 2014). Moreover, wollastonite typically results in pure by-products. The main by-products of its reaction are silica (SiO_2) and $CaCO_3$ (Kelemen et al., 2020). This contrasts with the carbonation of olivine and basalt, which often results in more complex mixtures of silicate minerals and metal oxides, some of which may not have immediate commercial value and could require additional processing or disposal (Gadikota et al., 2014;

Kelemen et al., 2020). In this study, wollastonite is considered as the emerging raw material to sequester CO_2.

To capture CO_2 using wollastonite through the process of mineral carbonation, we rely on the stoichiometry of the chemical reaction involved. The key reaction can be summarized as follows:

$$CaSiO_3 + CO_2 \rightarrow CaCO_3 + SiO_2$$

The stoichiometry of the reaction is 1:1 for wollastonite and carbon dioxide, meaning one mole of wollastonite reacts with one mole of CO_2 to produce one mole each of calcium carbonate and silicon dioxide. If we want to calculate the amount of CO_2 captured by 1 kg of wollastonite, the first step is converting the mass to moles which is:

$$\frac{1000\ g}{g/mole} = 8.61\ moles\ 116.165$$

The second step is to use the stoichiometry of the reaction. From the reaction equation, the stoichiometry between wollastonite and CO_2 is 1:1, meaning 1 mole of wollastonite reacts with 1 mole of CO_2 can produce 1 mole of $CaCO_3$. Thus, the moles of CO_2 that can be captured are equal to the moles of wollastonite calculated in Step 1, which is 8.61 moles. Then, convert the moles of CO_2 to mass. To find out how much CO_2 (in grams) can be captured, we use the molar mass of CO_2 (44.01 g/mol), and the mass of CO_2 equals moles of CO_2 (8.61 mols) times the molar mass of CO_2. The total mass of CO_2 captured by 1 kg of wollastonite is 378.86 grams (0.38 kg). These calculations show how much CO_2 can be sequestered by reacting with 1 kg of wollastonite under ideal conditions.

Haque et al. (2019) conducted experiments on EW using wollastonite applied to cropland for carbon sequestration and plant growth promotion. In this study, the carbon capture rate was 12.04 kg of CO_2/ton soil/month, with 0.125 tons (125 kg) of wollastonite used per ton of soil. Therefore, the annual carbon sequester rate is 144.18 kg of CO_2/ton of soil. When converted to the capture rate based on the weight of wollastonite, approximately 0.913 kg of CO_2 can be sequestered per kg of wollastonite used annually. Compared to the result under ideal conditions using the stoichiometric method, the experiment result is 2.42 times higher. I think the reason that experimental result has higher removal rate than ideal one because the wollastonite used in experiment is not pure. The composition of this nature wollastonite (extracted from Canadian Wollastonite's Ontario mine) that used in this study includes 55% of SiO_2, 26% CaO (present as wollastonite), 9% of MgO (present as diopside), and 10% of other elements. Therefore, not only wollastonite can react with CO_2 to produce final dissolved products, but also the MgO can indeed capture CO_2 from the air to form magnesium carbonate ($MgCO_3$) in a process known as carbonation. In addition, the pH of the environment is a crucial factor in the efficiency of CO_2 removal using enhanced weathering technology. The pH of the solution affects the speciation of TIC. At lower pH (more acidic conditions), CO_2 is more prevalent, while at higher pH (more alkaline conditions), bicarbonate and carbonate ions dominate. The optimal pH for wollastonite dissolution and subsequent carbonation typically lies in the neutral to slightly alkaline range, where both CO_2 and bicarbonate are available for reaction. Therefore, the suitable pH environment in this study (between 6.5 – 7.3) helps to improve the efficiency of carbon sequestration.

In 2022, the U.S. Geological Survey (2022) reported that global reserves of wollastonite are estimated to exceed 100 million tons. According to Peres et al. (2022), wollastonite can achieve a CO_2 sequestration efficiency of 82%. However, for example, to sequester the global CO_2 emissions of 36.1 Gt per year in 2022 with wollastonite at 82% sequestration efficiency under ideal conditions based on the stoichiometry method, approximately 116 billion tons of wollastonite would be required annually. Both estimations take into account the effective carbon sequestration capability of wollastonite, demonstrating that the amount needed vastly exceeds the reported global reserves of 100 million tons. This illustrates that while wollastonite is effective for CO_2 sequestration on a smaller scale or in specific contexts, it is not feasible for tackling global CO_2 emissions due to its limited availability compared to the massive requirements.

Basalt and olivine are two common silicate rocks used as raw materials for capturing CO_2 from the air through EW. Basalt is a dark-colored, fine-grained igneous rock predominantly composed of plagioclase and pyroxene. It is one of the most common types of rock on Earth, particularly on the ocean floors (Schmincke, 2003). The exact chemical composition of basalt can vary depending on its source and composition, but here is a typical breakdown of the major components by weight: 45-55% silicon dioxide (SiO_2), 14-18% aluminum oxide (Al_2O_3), 1018% iron oxide (include both FeO and Fe_2O_3), 10-18% calcium oxide (CaO), 8-12% magnesium oxide (MgO), 5-12% sodium oxide (Na_2O), 2-3.5% potassium oxide (K_2O), <1.2% titanium dioxide (TiO_2), 1-2% phosphorus, and 0.1-0.5% pentoxide (P_2O_5) (Winter, 2010). More than 90% of the volcanic rock found on Earth is composed of basalt, especially the oceanic crust alone contains about 2.9×10^9 km^3 (equals to 2.9×10^9 Gt) of basalt (Winter, 2010). Goll et al.

(2021) reported that 1 ton of basalt applied in hinterlands can remove 1.3 tons of CO_2 annually. Using the carbon emissions from 2022 as an example, approximately 27.77 billion tons of basalt would be required each year to sequester 36.1 Gt of CO_2. Olivine is a magnesium (Mg)-rich or iron (Fe)-rich silicate mineral used to sequester CO_2, and the general chemical formula is Mg_2SiO_4 or Fe_2SiO_4. Based on the stoichiometric method for reacting Mg_2SiO_4 with CO_2, the chemical reaction equation is as follows:

$$Mg_2SiO_4 + 2CO_2 \rightarrow 2MgCO_3 + SiO_2$$

The stoichiometry of the reaction is 1:2 for olivine and carbon dioxide, meaning that 1 mole of olivine reacts with 2 moles of CO_2 producing 2 moles of magnesite ($MgCO_3$) and 1 mole of SiO_2. Thus, 140.73 tons of olivine can absorb 88.02 tons of CO_2. Therefore, based on the efficiency where each ton of olivine can sequester approximately 0.625 tons of CO_2, about 57.76 billion tons of olivine would be required annually to remove 36.1 Gt of CO_2 in 2022, using this year as an example. Although there is no specific figure for the reserves of olivine, approximately 50% of the Earth's crust is covered by olivine (Mcdonough and Rudnick, 1998). Therefore, the quantity of available olivine is high enough to remove CO_2 from the air. In conclusion, while wollastonite is efficient but limited by availability, basalt offers a balance of moderate efficiency and abundant availability, making it a practical option for enhanced weathering projects. Olivine stands out for its potential vast reserves and favorable chemical properties, positioning it as potentially the most viable option for global-scale CO_2 sequestration, assuming logistical and environmental challenges can be effectively managed. Each material's suitability ultimately depends on a combination of scientific, logistical, and environmental considerations.

In the broader context of carbon sequestration, the utilization of wollastonite in carbon sequestration aligns with global initiatives aimed at combating climate change by reducing atmospheric CO_2 levels. As countries worldwide strive to meet the ambitious targets set by international agreements like the Paris Agreement, wollastonite offers a promising technique for CDR. By chemically reacting with CO_2 to form stable carbonates, wollastonite facilitates a permanent removal of this greenhouse gas from the atmosphere. This method not only contributes to the direct reduction of atmospheric CO_2 but also complements other carbon management strategies, such as renewable energy adoption and energy efficiency improvements. The integration of wollastonite into a broader carbon management framework can help nations achieve their net-zero emissions goals, enhancing the global response to climate change challenges. Furthermore, the application of wollastonite in carbon sequestration can have a transformative impact on industries responsible for high levels of CO2 emissions, such as the cement and steel industries. By integrating wollastonite into industrial processes, these sectors can significantly reduce their carbon footprint. The mineral's ability to sequester carbon during the production process offers an innovative way to decrease emissions from some of the most challenging sources. This industrial application not only aids in mitigating climate change but also promotes technological innovation and development within key sectors, driving economic growth while reducing environmental impacts. As such, wollastonite becomes a critical component of sustainable industrial practices, demonstrating the potential for industrial symbiosis where waste materials are repurposed for environmental benefit. However, the global impact of wollastonite usage for carbon sequestration depends heavily on its scalability and the logistical feasibility of its deployment on a large scale. Assessing the environmental impacts of mining, processing, and distributing wollastonite at the required volumes is crucial for understanding the overall benefits and potential drawbacks of this approach. Effective global implementation would require international cooperation to manage supply chains, harmonize regulatory standards, and share best practices and technologies. By fostering collaborative efforts and ensuring responsible management practices, the use of wollastonite in carbon sequestration can significantly contribute to global climate mitigation efforts, helping to stabilize global temperatures and foster a sustainable future.

The work on estimating the environmental impacts of using wollastonite provides critical insights that could significantly influence how we approach global strategies to mitigate climate change. This analysis not only evaluates the direct benefits of carbon dioxide reduction through the mineralization process but also considers the full environmental footprint of this approach, from extraction to application. When applying a life cycle assessment (LCA) to compare natural and synthesized wollastonite, the assessment framework provides a holistic view of the environmental impacts from the initial extraction or synthesis to the final application in carbon sequestration. For natural wollastonite, the LCA would track impacts from the extraction phase, which includes mining operations that can disrupt local ecosystems and landscape, and processing steps, which often involve crushing and milling the mineral. These processes consume significant amounts of energy and can emit particulate matter and other pollutants. Additionally, the transportation of natural wollastonite from mine sites to places of use must be considered, as it contributes to fossil fuel consumption and greenhouse gas emissions depending on the distance and mode of transport used. In contrast, the LCA for synthesized wollastonite focuses on the manufacturing process, which involves high-temperature reactions between silica and calcium carbonate. This synthetic process is energy-intensive, with most of the energy typically derived from non-renewable sources unless renewable energy solutions are integrated into the production process. Furthermore, while the synthesis process allows for the creation of a purer and more uniform product, which can be advantageous for consistent carbon sequestration outcomes, it also necessitates a careful evaluation of the trade-offs between the higher energy requirements and the benefits of product homogeneity and performance. In this study, using natural wollastonite as the raw material for carbon sequestration is identified as a negative carbon technique, whereas using synthesized wollastonite results in higher carbon emissions than those it captures. However, in this study, several factors are not considered. An LCA comparison of natural and synthesized wollastonite needs to consider the potential for material reuse or recycling. Natural wollastonite, used in soil amendments for agriculture, not only sequesters carbon but also delivers agronomic benefits, which may enhance the soil's natural carbon capture over time. Synthesized wollastonite might offer similar benefits if applied in the same context, but its environmental justification must also account for the recycling or disposal of industrial by-products produced during its manufacture. The reuse of materials in the wollastonite synthesis process could mitigate some environmental impacts, highlighting the need for innovative approaches to maximize material efficiency and minimize waste. In addition, the water consumption required for irrigation to support plant growth should also be considered. By evaluating all these factors, LCA provides critical insights that guide decision-making toward the most environmentally sustainable choices for carbon sequestration using wollastonite.

The establishment of stringent regulations and incentives is vital for optimizing the use of mineral rocks in carbon sequestration projects. Governments have the opportunity to set robust quality standards that dictate the purity and particle size of minerals necessary for effective carbon capture. By ensuring that the minerals used in these projects meets specific criteria, the efficacy of the carbon sequestration process can be maximized while minimizing the need for energy-intensive processing. Additionally, regulations can enforce sustainable mining practices that minimize environmental impact, such as requiring the restoration of mined areas and the implementation of best practices for water management and dust control. These regulations not only protect the environment but also ensure that the use of wollastonite contributes positively to carbon dioxide reduction efforts. In addition, financial incentives play a crucial role in advancing the use of minerals for carbon sequestration by making it economically viable for companies to invest in the necessary technologies and practices. For instance, innovations that allow for the extraction of mineral rocks with reduced energy consumption or that improve the carbonation process would make the overall carbon sequestration method more sustainable. Furthermore, tax breaks or subsidies for companies that source minerals locally can significantly reduce transportation emissions associated with moving this material from the mine to application sites. Such financial incentives not only encourage the adoption of green technologies but also support the growth of an industry that contributes to the mitigation of climate change. To ensure the successful integration of these regulations and incentives, a collaborative approach involving stakeholders from government, industry, and the scientific community is essential. Regular reviews and updates to policies based on the latest scientific findings and technological advancements will help maintain the relevance and effectiveness of these measures. Moreover, clear communication of these policies and the benefits they aim to provide will help obtain public and corporate support, ensuring widespread uptake and compliance. These regulatory and financial strategies form a comprehensive framework that supports the responsible and beneficial use of minerals in addressing one of the most pressing global challenges.

1.5.2. Chapter 3

In this study, CO_2 is considered as feedstock to produce bioplastic (e.g., polyhydroxybutyrate (PHB)) via electrochemical and bio-synthesis processes. The data for electrochemical and biosynthesis processes are from Rice University and the University of California, Los Angeles, respectively. The system boundary is a "cradle-to-gate" assessment, including raw materials extraction of both processes and the production phase. For the electrochemical process, the production of highly pure acetate is successfully achieved through the process of electrocatalytic CO reduction (CORR). This transformation provides new possibilities for using CO gas to create valuable products.

Carbon capture, utilization, and storage (CCUS) technologies encompass a range of techniques and processes designed to capture CO_2 emissions from sources like power plants and industrial processes, or directly from the atmosphere, and either reuse it or store it so it won't enter the atmosphere. CCUS are seen as crucial technologies in efforts to combat climate change by reducing greenhouse gas emissions and are often considered in strategies to achieve net-zero emissions. CCUS technologies are divided into carbon capture technologies, carbon utilization technologies, and carbon storage technologies. The carbon capture technological pathways include post-combustion, pre-combustion, oxy-fuel combustion, and direct air capture (DAC) systems. Pre-combustion capture involves removing CO_2 from fossil fuels before combustion is completed. This method typically converts fuel into a mixture of hydrogen and carbon dioxide, from which CO_2 can be separated and captured before the hydrogen is burned as a clean fuel. Physical or chemical absorption techniques are typically used for pre-combustion capture. Precombustion is a more energy-intensive process compared to other capture technologies for the gasification process and the subsequent separation of CO_2 from the syngas. Post-combustion capture, the most widely adopted method, involves capturing CO_2 from the flue gases produced by combustion. This is done using various technologies, such as chemical solvents, which absorb CO_2 from the exhaust. Meanwhile, oxy-fuel combustion is a process that burns fuel in pure oxygen instead of air, resulting in flue gases composed primarily of CO_2 and water vapor, simplifying the capture process. Aside from these traditional methods, DAC represents a cutting edge approach that involves capturing CO_2 directly from ambient air. DAC technologies are particularly compelling because they can be deployed anywhere, unlike other methods that need to be connected to specific CO_2 sources. This flexibility makes DAC an attractive option for offsetting emissions from sectors that are difficult to decarbonize, such as agriculture and aviation. However, DAC is energy-intensive and currently costly, highlighting the need for ongoing research and development to improve its efficiency and affordability. As global efforts to combat climate change intensify, the role of carbon capture technologies, including DAC, is expected to become more critical, offering a viable pathway to achieving net-zero emissions while supporting continued economic growth. According to the summary from Yagmur Goren et al. (2024), DAC has a higher energy requirement for carbon capturing compared to precombustion, post-combustion, and oxy-combustion regardless of capturing efficiency. In addition, despite being an energy-intensive process, oxy-combustion has the lowest global warming potential (GWP) among CO_2 capture technologies, due to its relatively lower energy consumption and no need for chemical agents. Besides, the energy consumption will be decreased if the oxygen purity increases for the oxy-combustion method. In my opinion, considering the carbon capture technologies for extracting waste CO_2 from power plants or industrial processes as a raw material for bioplastic production, the oxy-combustion method should be selected due to its lower energy consumption and carbon emissions.

Negative Emissions Technologies (NETs) represent a crucial suite of innovations aimed at combating climate change by removing CO_2 from the atmosphere and securely storing it. As global temperatures continue to rise due to the persistent increase in greenhouse gases, the role of NETs becomes increasingly vital. These technologies not only complement efforts to reduce emissions but also provide a means to achieve net-negative emissions, which is essential for limiting global warming to safe levels. The diverse array of NETs offers various approaches, each with unique mechanisms and benefits, thereby enhancing the overall robustness and adaptability of climate mitigation strategies. DAC and Bioenergy with Carbon Capture and Storage (BECCS) are two prominent NETs that have gained significant attention. DAC has been introduced in the previous paragraph. BECCS combines biomass energy production with CO_2 capture and storage, effectively creating a cycle that removes CO_2 from the atmosphere while generating renewable energy. These technologies underscore the innovative approaches being developed to address the urgent need for carbon removal. Natural-based solutions such as afforestation and reforestation, and enhanced weathering also play a pivotal role in NETs. Afforestation and reforestation involve planting new forests or restoring existing ones, leveraging the natural process of photosynthesis to absorb CO_2. Enhanced weathering is one of soil carbon sequestration methods that focuses on enhancing the carbon storage capacity of soils through agricultural practices like no-till farming and cover cropping. This method not only contribute to carbon removal but also offer additional environmental benefits, such as biodiversity conservation, improved soil health, and water regulation. Marine and geological NETs, including ocean fertilization, ocean alkalinity enhancement, and carbon mineralization, expand the scope of carbon removal strategies. Ocean fertilization aims to boost the growth of phytoplankton, which absorb CO_2 and transport it to the deep ocean upon their death. Ocean alkalinity enhancement involves adding alkaline substances to seawater to increase its CO_2 absorption capacity. Carbon mineralization accelerates the natural process of forming stable carbonates by reacting CO_2 with minerals, providing a durable form of carbon storage. Biochar is a form of charcoal produced from organic waste materials through a process called pyrolysis, which involves heating the biomass in the absence of oxygen. This technology not only provides a stable way to sequester carbon but also enhances soil health and fertility. When added to soils, biochar can significantly improve water retention, nutrient availability, and microbial activity, leading to more sustainable agricultural practices. By converting organic waste into a longlasting carbon storage medium, biochar helps reduce greenhouse gas emissions, contributing to climate change mitigation efforts. These diverse approaches illustrate the multifaceted nature of NETs and their potential to significantly mitigate climate change through innovative and integrated solutions. Figure 1 presented the carbon emissions associated with various NETs, measured in tons of CO_2 emitted per ton of CO_2 sequestered and all the numbers are averaged. DAC has the highest emission ratio, with approximately 0.7 tons of CO_2 emitted per ton of CO_2 sequestered (Fasihi et al., 2019; Keith et al., 2018). BECCS follows, emitting around 0.3 tons of CO_2 per ton sequestered (Sanchez et al., 2015). Afforestation and reforestation and ocean alkalinity enhancement show significantly lower emissions, with less than 0.1 tons of CO_2 (Griscom et al., 2017; Renforth and Henderson, 2017). The rest of technologies, including ocean fertilization, carbon mineralization, biochar, and enhanced weathering, present moderate emissions (between 0.1 to 0.2 tons of CO_2 per ton sequestered) (Beerling et al., 2020a; Matter and Kelemen, 2009; Woolf et al., 2010). Therefore, the DAC is not recommended for carbon capture compared to other technologies due to the high energy consumption.

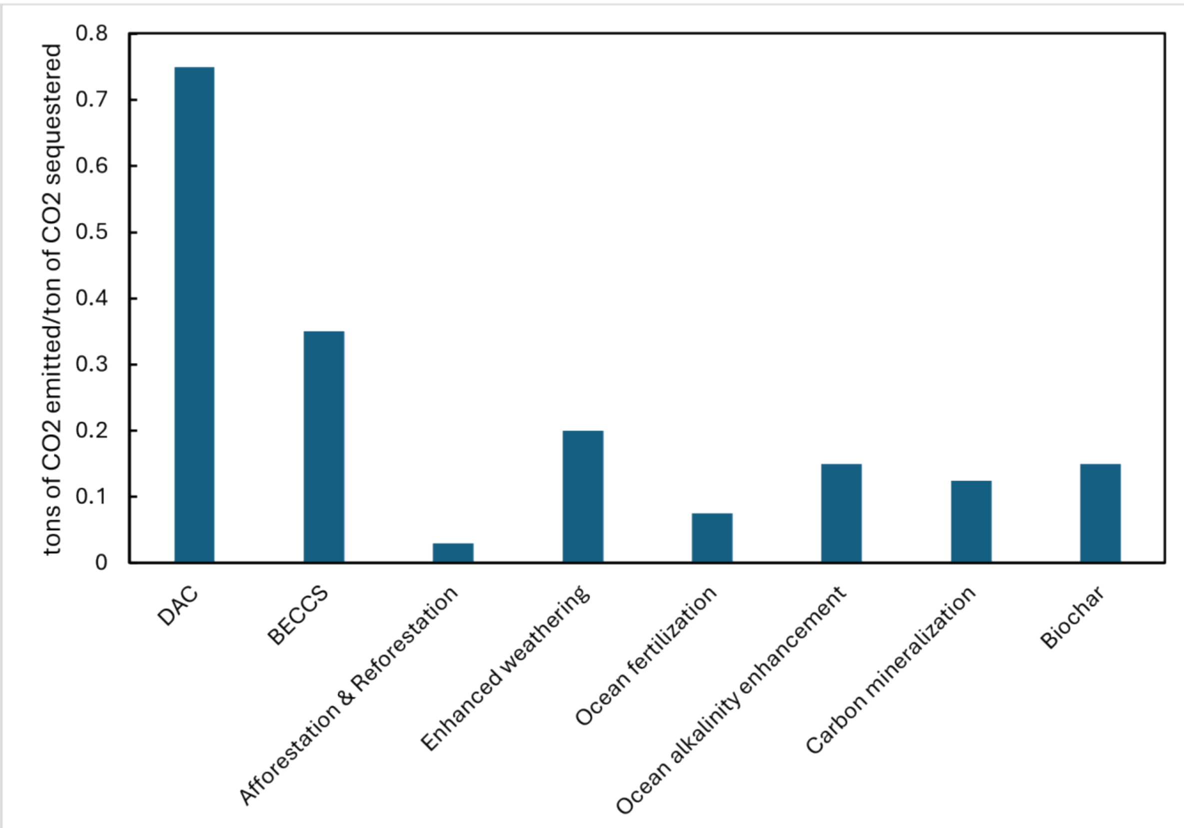

Figure 3. The carbon emission comparison of NETs for 1 ton of CO_2 sequestered (all the numbers are averaged.) (Beerling et al., 2020a; Fasihi et al., 2019; Griscom et al., 2017; Keith et al., 2018; Matter and Kelemen, 2009; Renforth and Henderson, 2017; Sanchez et al., 2015; Woolf et al., 2010)

Carbon capture and utilization (CCU) technologies are used captured CO_2 from atmosphere or industrial processes as a raw material to produce valuable products (Otto et al., 2015). Unlike CCS, where the captured CO_2 is stored underground, CCU focuses on reusing CO_2 as a raw material in various industrial applications (Sharifian et al., 2021). This not only helps in reducing the overall CO_2 emissions but also provides economic incentives by creating commercially viable products from waste CO_2 (Hepburn et al., 2019). The integration of CCU technologies into existing industrial processes can significantly contribute to the development of a circular carbon economy, where carbon is continuously recycled and utilized (Naims, 2016). One of the primary methods of CCU is chemical conversion, where captured CO_2 is transformed into synthetic fuels and chemicals (Aresta et al., 2013). This process often involves using renewable energy sources to power chemical reactions that convert CO_2 into hydrocarbons like methanol, ethanol, and other fuels (Olah et al., 2009). These synthetic fuels can be used as alternatives to fossil fuels, thus reducing the carbon footprint of transportation and other sectors (Artz et al., 2018; Dufour et al., 2012). By transforming CO_2 into useful products, chemical conversion not only mitigates emissions but also supports the production of sustainable and eco-friendly materials. Another promising area of CCU is biological and mineralization processes. In biological conversion, CO_2 is used to cultivate microalgae, which can then be processed into biofuels, animal feed, and other bioproducts (Razzak et al., 2013). This method not only sequesters CO_2 but also provides a sustainable source of biomass (Chisti, 2007). Enhanced plant growth in greenhouses using CO_2 can improve agricultural productivity, contributing to food security and sustainability (Beal et al., 2015). In mineralization, CO_2 reacts with minerals or industrial wastes to produce construction materials like concrete and aggregates (An et al., 2019). This not only locks away CO_2 in a stable form but also creates durable building products, reducing the demand for traditional, carbon-intensive construction materials. Electrochemical conversion is another innovation CCU technology. This process utilizes electricity to convert CO_2 into carbon monoxide (CO) and oxygen (O_2), which can then be used to produce synthetic fuels and chemicals, such as acetic acid and formic acid (Zhu et al., 2021). However, the electrochemical process has high energy consumption, regardless of whether it involves CO_2 conversion or electrolysis processes. Therefore, the renewable alternatives (e.g., wind, solar) are more sustainable energy resources to substitute conventional resources for electricity generation in order to achieve net-negative emissions. Previous studies have quantified the carbon emissions associated with various CCU products. The carbon emissions associated with various CCU products vary depending on the specific processes and energy sources used. Synthetic fuels, such as methanol and ethanol, typically emit around 0.2 to 0.5 tons of CO_2 per ton of CO_2 utilized, largely influenced by the energy source and process efficiency (Hepburn et al., 2019; Rigamonti and Brivio, 2022). Chemicals like urea, formic acid, and polycarbonates generally have emissions between 0.1 to 0.3 tons of CO_2 per ton of CO_2 utilized (Artz et al., 2018). The cultivation of microalgae for biofuels can result in emissions as high as 1.5 to 2 tons of CO_2 per ton of CO_2 utilized, especially when powered by renewable energy (Zieliński et al., 2023). Producing building materials such as concrete and aggregates through mineralization processes emits about 0.1 to 0.8 tons of CO_2 per ton of CO_2 utilized based on the different carbon capture technologies (An et al., 2019). Electrochemical conversion products, including carbon monoxide and synthetic fuels, have emissions ranging from 0.2 to 0.4 tons of CO_2 per ton of CO_2 utilized, depending on the energy source (Somoza-Tornos et al., 2021). Enhanced oil recovery has significant emissions, with the high emission scenario reaching 1.0 tons per ton of CO_2 utilized, indicating it may not be carbon-negative overall (Alam et al., 2022). These estimates highlight the importance of energy sources and process efficiencies in determining the overall carbon footprint of CCU products, with advancements and increased use of renewable energy expected to further reduce emissions over time. Most of the CCU products are carbon negative. The final carbon emissions of CO_2-based products are various because the energy consumption and amount of CO_2 needed for product manufacturing are different. Therefore, we should consider more sustainable solutions to reduce the carbon emissions, such as improving technology efficiencies and using renewable energy.

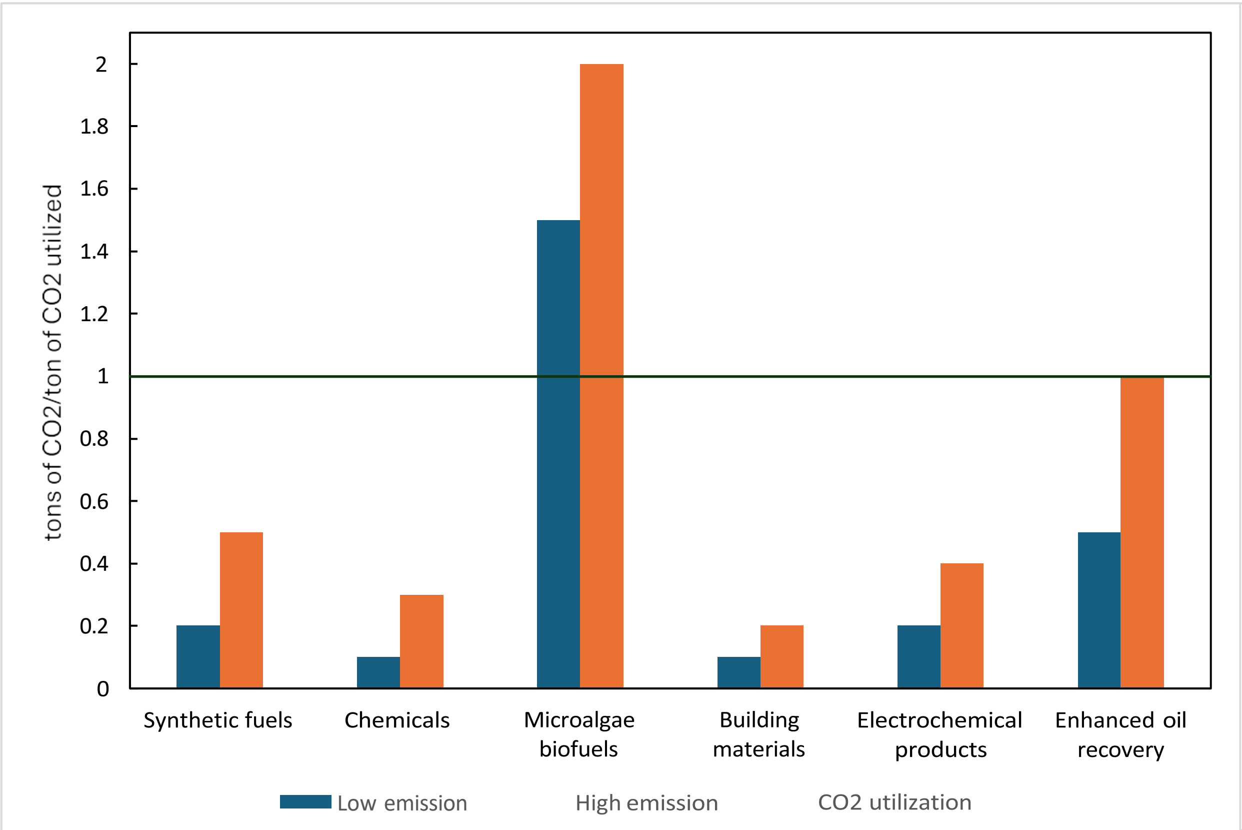

Figure 4. The compared carbon emissions of CCU products for 1 ton of CO_2 utilized (Alam et al., 2022; An et al., 2019; Artz et al., 2018; Hepburn et al., 2019; Rigamonti and Brivio, 2022; Somoza-Tornos et al., 2021; Zieliński et al., 2023).

Polyhydroxybutyrate (PHB) is a type of bioplastic that can be produced from various raw materials to substitute the conventional plastics. The primary feedstocks for PHB production include CO_2, glucose from corn, lignocellulosic materials, and wastewater. This project aims to integrate electrochemical and bio-synthesis processes to produce bioplastic (PHB) using CO_2 as raw material. Figure 3 illustrates the carbon emissions to produce 1 kg of PHB from various feedstocks. PHB production using CO_2 with CO conversion shows the highest emissions, approximately 40 kg CO_2 eq/kg PHB produced. This finding indicates that the conversion process involving CO is highly energy-intensive and contributes substantially to the overall emissions. In comparison, using CO_2 directly and without CO conversion processes results in minimal emissions (0.38 kg CO_2 eq/kg PHB produced), emphasizing the potential of this method as a low-carbon alternative for PHB production although not truly carbon negative. The other feedstocks, including glucose from corn, lignocellulosic, and wastewater, have moderate emissions ranging from approximately 4 – 8 kg CO_2 eq/kg PHB produced (Fernández-Dacosta et al., 2015; Kookos et al., 2019; Nieder-Heitmann et al., 2019). These values are relatively lower compared to the CO_2 with CO conversion method but still indicate significant environmental impacts, primarily due to the energy and processing requirements involved in converting these materials into PHB. Conventional PET production, included as a reference, shows emissions comparable to the lower end of these methods (2.15 kg CO_2 eq/kg PHB produced), reinforcing the need for sustainable bioplastic alternatives (Tamburini et al., 2021). Therefore, the results demonstrate that the PHB production using CO_2 as raw material without CO conversion is not carbon negative. However, compared to other raw materials, using CO_2 directly without any conversion processes has environmental benefits. This feedstock can be considered as alternative to replace glucose, lignocellulosic, and wastewater for bioplastic production. I think if the production processes have to involve CO_2 conversion into CO, renewable energy resources should be utilized to decrease the carbon emissions during manufacturing due to the high energy consumption.

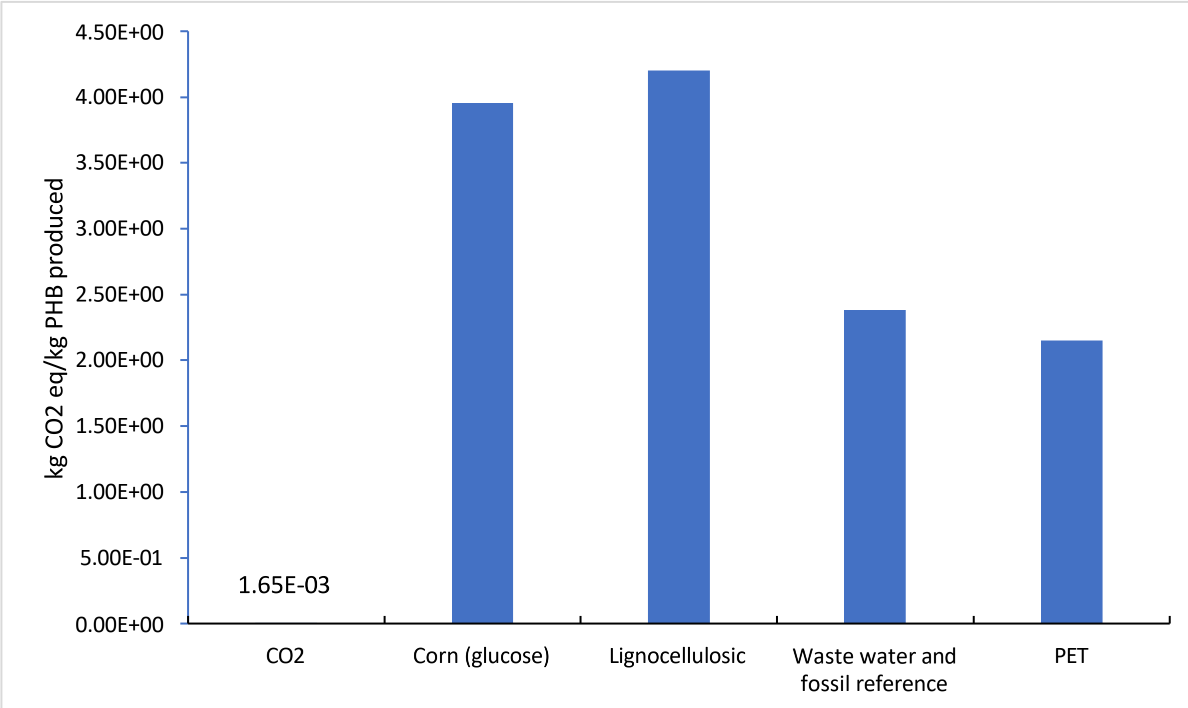

Figure 5. The carbon emission of PHB production based on various raw materials (FernándezDacosta et al., 2015; Kookos et al., 2019; Nieder-Heitmann et al., 2019; Tamburini et al., 2021). Note: the results of carbon emissions using CO_2 as feedstock with and without CO production are from my LCA study.

Switching to CO_2-derived bioplastics for single-use plastic water bottles in the U.S. presents a compelling environmental initiative due to its potential to utilize atmospheric CO_2, a major greenhouse gas. This approach aligns with carbon capture and utilization strategies, especially electrochemical and bio-synthesis processes, potentially reducing the net carbon footprint of plastic production. Based on the LCA results, using CO_2 as feedstock directly to produce single use bioplastic has better environmental performance compared to other raw materials for bioplastic production. However, the feasibility of this switch heavily depends on the energy sources used in the production process. The findings illustrate that the electrochemical process has higher environmental implications during manufacturing. If renewable energy sources are employed, the environmental benefits are maximized, contrasting sharply with the current high carbon emissions associated with conventional fossil-based plastic production and other bioplastic feedstocks. Besides, the technological maturity and scalability of CO_2-derived bioplastics are still under development, which could limit their immediate application on a large scale. The efficiency for acetic acid conversion from CO or CO_2 is essential to scale up the bioplastic production to commercial scale. From cost perspective, CO_2-derived bioplastics, being in the early stages of commercial development, often entail higher initial capital investments for setting up the necessary technology and equipment. These are typically more advanced and costly due to the complexity required in capturing and polymerizing CO_2. Additionally, operational costs are likely higher due to the energy-intensive nature of CO_2 conversion processes, which could be further compounded if the energy used is derived from non-renewable sources. Bioplastics derived from agricultural products offer another alternative, utilizing renewable resources such as corn or sugarcane. These materials not only help reduce reliance on fossil fuels but also biodegrade more readily than conventional plastics. However, their production competes with food resources and can lead to other environmental issues such as increased use of water, fertilizers, and pesticides. Additionally, similar to CO_2-derived plastics, the total environmental benefit of agricultural bioplastics depends on the lifecycle analysis, which considers factors from cultivation to product end-of-life. This analysis often reveals tradeoffs between reducing carbon emissions and impacting other aspects of environmental sustainability, such as water consumption and biodiversity. In contrast, conventional fossil-based plastic water bottles have significant environmental implications, while economically favorable due to established production techniques and lower costs. These plastics contribute substantially to carbon emissions during production and pose long-term environmental hazards due to their non-biodegradable characteristic. The widely use of fossil-based materials has led to ecological damage, notably in marine environments, highlighting the urgent need for alternatives that mitigate these impacts. Overall, CO_2-based bioplastic single-use water bottles offer a promising alternative that could achieve environmental sustainability goals, especially if renewable energy sources are used in production processes. However, cost, scalability, and technological development need to be considered to assess the full potential and practicality of implementing such a change on a commercial scale.

1.5.3. Chapter 4

In recent years, bio-based plastic has seen significant evolution, driven by an increasing awareness of environmental issues and a growing demand from consumers for sustainable alternatives to conventional petroleum-based plastics. The innovative use of captured CO_2 as a raw material in the production of bioplastics represents a significant shift towards more sustainable manufacturing practices. By converting a greenhouse gas into a usable product, this approach aims to help in reducing the environmental impact associated with traditional plastic production, and it is important to note that the PHB synthesis process without CO production can be less environmentally impactful than using other bioplastic feedstocks (e.g., corn) and petroleum-based plastics (e.g., PET). Based on this, this production approach contributes to the broader climate change mitigation efforts. However, the bioplastic products market experienced limitation for growth and competition due to the higher production cost and limited availability.

Therefore, understanding consumer willingness to pay for CO_2-based bioplastic bottles is crucial for scaling up this technology and making it commercially viable.

Our research focused on the development and consumer acceptance of single-use water bottles made from CO_2-based bioplastics, a precursive approach that utilizes captured CO_2 as a primary raw material via electrochemical and bio-synthesis processes. The objective of this study was to evaluate the feasibility of producing bioplastic products from sequestered CO_2 and to assess consumer willingness to pay (WTP) for these environmentally innovative products. Methodologically, we used survey approaches to estimate consumer reactions and price sensitivity. Our research findings on CO_2-based bioplastics are closely aligned with existing literature on consumer willingness to pay (WTP) for biobased products, which consistently shows a positive correlation between environmental benefits and increased consumer spending. Previous studies highlighted that consumers are more likely to invest in products that they perceive as directly contributing to environmental sustainability (De Marchi et al., 2020a; Scherer et al., 2018; Skouloudis et al., 2023; Zwicker et al., 2023a). In our study, CO_2-based bioplastics were particularly notable for their reduced carbon footprint, which is a critical factor given the increasing public concern over carbon emissions and climate change. By transforming CO_2 into useful products from industrial processes, these bioplastics not only prevent the release of greenhouse gases but also utilize them constructively, which significantly attracts to eco-conscious consumers. Additionally, the potential for recycling and the novelty of CO_2-based bioplastics are attributes that further influence consumer WTP. The ability to recycle these products at the end of their lifecycle resonates well with current trends favoring circular economy principles, where the goal is to maximize resource efficiency and minimize waste. This attribute ensures that CO_2-based bioplastics maintain value even after use, enhancing their attraction compared to traditional plastics, which often end up in landfills. Furthermore, the novelty of using captured CO_2 as a raw material in consumer products provides a unique selling point that can attract consumers interested in innovative solutions to environmental problems. Our findings contribute new insights into the WTP literature by demonstrating that the specific environmental benefits associated with CO_2-based bioplastics, such as their role in reducing industrial carbon footprints and potential for recyclability, can significantly enhance consumer valuation of these products. These insights suggest that as consumer awareness of environmental issues continues to grow, there is substantial market potential for bioplastics that effectively communicate their ecological advantages. Thus, our research emphasizes the importance of marketing strategies that focus on educating consumers about the environmental impact of their purchases and the benefits of choosing products made from CO_2-based bioplastics. This approach not only facilitates greater consumer engagement but also promotes a broader shift towards sustainable consumption practices.

Once CO_2-based plastics are produced at scale, several specific benefits may occur. From environmental perspective, the integration of CO_2-based plastics into the market promotes a more sustainable lifecycle for plastic products. By converting waste CO_2 into a valuable resource, the process supports a circular economy, where materials are continually reused and recycled. Additionally, the production of CO_2-based plastics reduces the need for these fossil fuels, as the primary raw material is captured carbon dioxide. This shift not only conserves nonrenewable resources but also minimizes the environmental impacts associated with fossil fuel extraction, such as habitat destruction, water pollution, and oil spills. From the social perspective, large-scale production of CO_2-based plastics can lead to increased consumer acceptance, market differentiation, cost reductions, enhanced perceived value, and positive CSR impacts, all contributing to a greater willingness to pay for sustainable plastic alternatives.

The WTP results indicated the potential market viability of bio-based products. Even the biobased alternatives have higher production costs due to the unmature technologies in commercial scale compared to the conventional products. However, the most consumers prefer to purchase sustainable products even the price is higher. Therefore, the technologies development for sustainable products manufacturing are significant in order to reduce the initial costs for production. Companies and investors considering the production and commercialization of bioplastics can reference these findings as a favorable indication that there exists a market segment that places a high value on sustainability. This insight might motivate more companies to investigate and expand their offerings of innovative and sustainable products, aware that there is a dedicated consumer base that endorses initiatives. This awareness can simulate businesses to increase their investments in eco-friendly technologies and products, capitalizing on the support from environmentally conscious consumers.

Meanwhile, the findings from this study offer valuable insights that can significantly influence policy-making and business strategies aimed at enhancing the market penetration of biobased products. Policymakers, recognizing the environmental and economic benefits of bioplastics, can play a pivotal role by implementing supportive frameworks that encourage their development and adoption. One effective strategy could be the introduction of subsidies or tax incentives for manufacturers that invest in bioplastic production facilities or research and development. Such financial incentives can lower the entry barriers for new firms and reduce production costs, making biobased products more competitive against conventional plastics. Additionally, government policies that mandate the use of sustainable materials in government procurement or public projects can create a stable demand, encouraging further investment and industry growth. For businesses, strategic pricing adjustments and targeted marketing campaigns are essential to capitalize on the growing consumer interest in sustainable products. Pricing strategies should consider the premium consumers are willing to pay for environmentally friendly products, as demonstrated by the willingness to pay data. However, it is crucial for these prices to be balanced with the perceived value of the sustainability benefits. Marketing campaigns, on the other hand, should focus on educating consumers about the specific environmental benefits of bioplastics, such as reduced carbon emissions and better end-of-life disposal options. Highlighting these attributes can enhance consumer perception of biobased products and drive purchase decisions. Businesses could also benefit from collaborations with environmental organizations to encourage their sustainability credentials and gain consumer trust. Moreover, the synergy between government policies and corporate strategies can create a beneficial environment for the adoption of biobased products. Relevant departments can support innovations in bioplastic production not only through direct financial aids but also via regulatory measures that support sustainable products. For example, implementing stricter regulations on carbon emissions and waste production can indirectly promote the market for bioplastics by increasing the cost of non-compliant practices. Simultaneously, public awareness campaigns led by governments in partnership with private entities can raise the profile of biobased products, educating consumers about their benefits and reinforcing the social standard towards sustainable consumption. These coordinated efforts can significantly accelerate the transition towards a more sustainable plastic economy, reflecting a shared commitment to environmental management and innovation.

The societal impacts of adopting CO_2-based bioplastics are important. As public awareness and concern for environmental issues grow, consumer demand shifts towards more sustainable products, influencing market trends and corporate strategies. This transition supports the development of green technologies and industries, creating jobs and increasing economic growth within a sustainable framework. Additionally, the widespread use of bio-based bioplastics can lead to educational opportunities and community engagement in sustainability practices, reinforcing a collective environmental ethos among consumers and industries alike. By aligning economic activities with environmental conservation, the adoption of bio-based plastics not only addresses immediate ecological challenges but also contributes to building a resilient and sustainable society for future generations.

1.5.4. Chapter 5

This study utilized agent-based modeling (ABM) to estimate adoption rate of single-use carbon captured bioplastic water bottles compared with fossil-fuel based water bottles in the United States. ABM is a powerful tool for exploring the detailed dynamics of consumer behavior in market environments, particularly because of its ability to simulate individual-level interactions and decisions. This method excels in modeling the human behaviors and decision-making processes of consumers, where each agent can represent a unique individual with distinct characteristics, preferences, socioeconomic backgrounds, and levels of environmental consciousness. For instance, ABM can be used to represent a spectrum of consumers ranging from highly eco-conscious individuals willing to pay a premium for sustainable products to budget-conscious consumers who prioritize cost over environmental benefits. This diversity allows the model to capture a broad array of behaviors and demonstrate how individual consumer choices influence market trends. By applying distinct behavioral rules to each agent, ABM facilitates the simulation of complex social dynamics that significantly impact product adoption. For example, in the case of adopting sustainable products like carbon-captured bioplastic water bottles, ABM can illustrate how adoption can spread within a community. Agents programmed with a higher tendency to adopt based on peer recommendations might influence their network, creating a ripple effect where the adoption rate increases exponentially within certain clusters. Conversely, ABM can also show how negative perceptions or experiences shared within a social network can significantly prevent product adoption, demonstrating the critical role of positive endorsements and community acceptance. Moreover, ability of ABM is to model non-linear interactions and feedback loops adds depth to understanding market dynamics, which is particularly relevant for new product introductions like bioplastic water bottles. Nonlinear dynamics, such as when a small number of initial adopters triggers a larger communitywide shift towards a product, are precisely where ABM performs. It can simulate scenarios where initial slow adoption rates pick up speed as visibility increases or as certain market thresholds are met. Additionally, feedback loops within ABM allow the simulation of how consumer experiences with the product (positive or negative) feedback into the system, influencing future purchasing decisions and overall market penetration. These capabilities make ABM an indispensable tool for predicting market behavior, designing effective marketing strategies, and planning robust policy interventions to improve the adoption of sustainable practices. The depth and adaptability of ABM provide insights that are often beyond the scope of traditional deterministic models, making it an invaluable resource for researchers and policymakers dealing with complex, variable systems.

ABM offers a distinctive approach to understanding complex systems, fundamentally different from the insights provided by deterministic models. One of the most significant contributions of ABM is its ability to explain emergent phenomena. Emergence occurs when the interactions between individual agents following simple rules lead to complex behaviors and outcomes that are not explicitly programmed into the model. Different with deterministic models, where outcomes are directly and predictably derived from initial conditions without any emergence, ABM can capture the unexpected and often complex patterns that arise naturally from the microlevel dynamics of agent interactions. This capability is invaluable for understanding market trends and consumer dynamics, where individual decisions and social influences can lead to unpredictable collective behaviors, such as rapid shifts in market demand or sudden adoption of new technologies. These emergent phenomena are crucial for accurately reflecting real-world complexity and variability in modeling scenarios. In addition, capability of ABM for extensive scenario exploration and policy testing further distinguishes it from deterministic models. In ABM, researchers can simulate a wide range of scenarios by altering agent behaviors, environmental conditions, or policy settings and observing the resultant effects on the system. This flexibility allows for a detailed examination of how different interventions might play out in a dynamic market environment. For instance, ABM can be used to test the impact of various environmental regulatory or fiscal policies on the adoption rates of sustainable products like bioplastic water bottles. Researchers can modify parameters related to tax incentives, subsidy schemes, or public awareness activities and track how these changes influence consumer behavior and market penetration over time. This type of scenario testing is particularly beneficial for policymakers and strategists, providing them with a tool to predict the consequences of decisions before their implementation, which is a capability not typically afforded by deterministic models. Moreover, the aspect of adaptation and learning in ABM represents a significant advancement over deterministic approaches. Agents in an ABM can adjust their behaviors based on past experiences or changes in their environment, mimicking real-world learning and adaptation processes. This feature is especially relevant in markets and technologies where consumer preferences evolve in response to new information, technological advances, or changing social rules. For example, as more consumers become aware of the environmental impact of their purchases, they might shift their buying preference, which in turn influences the strategies of competitors and the overall market structure. Deterministic models often fail to capture this dynamic as they generally operate with fixed parameters that do not allow for behavioral changes over time. In contrast, ABM provides a dynamic framework where continuous learning and adaptation are integral to the model, offering a more realistic and responsive tool for analyzing complex systems where change is constant. These unique types of insights generated by ABM underscore its superiority in dealing with complex, adaptive systems where understanding the depth of individual actions and their interplay within a broader context is crucial. By leveraging ABM, researchers and decision-makers can gain a deeper, more actionable understanding of the systems they study or manage, making it an invaluable tool in the precious of modern computational modeling.

From the results of my ABM study on the adoption of single-use CO_2-based bioplastic water bottles, several key insights about real-world consumer behavior and market dynamics emerge. These findings not only enhance our understanding of what drives consumer choices but also provide valuable guidance for policymakers, manufacturers, and marketers aiming to increase the adoption of sustainable products. First, this study offers compelling evidence that economic and environmental factors are primary in influencing consumer decisions regarding the adoption of single-use CO_2-based bioplastic water bottles. Specifically, the findings indicate that both the cost of bioplastic water bottles and their environmental footprint (EF) are critical determinants of consumer preferences and adoption rates. When the costs associated with these bottles are lower, and their environmental impact is minimized, there is a marked increase in consumer willingness to adopt. This relationship underscores the dual influence of price sensitivity and environmental consciousness in consumer purchasing decisions, reflecting broader market trends where costefficiency and sustainability are key to product success. In practical terms, the study suggests that manufacturers and marketers aiming to increase the market penetration of bioplastic products must strategically address these two drivers. For cost-conscious consumers, demonstrating economic feasibility is crucial. This could involve simplifying production processes to reduce costs, achieving economies of scale, or implementing innovative technologies that lower the overall price point of bioplastic products without compromising quality. At the same time, for environmentally conscious consumers, it is essential to highlight the reduced environmental footprint of using bioplastics compared to conventional plastics. This can be achieved through transparent marketing strategies that clearly communicate the environmental benefits, such as lower CO_2 emissions, reduced fossil fuel usage, or improved recyclability compared to traditional plastic options. Moreover, these findings have implications for policy-making and consumer education. Policymakers could consider incentives for manufacturers that reduce the cost and environmental impact of bioplastic products, such as tax breaks, subsidies, or support for research and development. Consumer education activities can also play a pivotal role, informing the public about the benefits of bioplastics and how their choices can impact the environment. By aligning economic incentives with environmental benefits, strategies can be more effectively to enhance consumer uptake and support the broader transition towards sustainable consumer products. This deliciated understanding of the economic and environmental factors driving consumer behavior is crucial for developing targeted interventions that encourage the adoption of environmentally friendly products in a cost-sensitive market.

The findings illuminate an aspect of social dynamics within the adoption process of bioplastic water bottles, revealing a complex interplay between neighbor influence and adoption rates. Interestingly, while conventional wisdom and previous research often suggest that increased social interaction within communities generally promotes the adoption of new products, the results of this study indicate otherwise for bioplastic bottles. Specifically, an increase in neighbor influence is correlated with lower adoption rates. This counterintuitive finding suggests that the nature of social influence in this context may not always be straightforward or positive. This conflictive outcome could be attributed to several factors inherent in the dynamics of social influence. In some communities, heightened discussions about bioplastic bottles may inadvertently focus on potential drawbacks rather than benefits, especially if these conversations are driven by skepticism or misinformation. For instance, concerns about the cost, effectiveness, or aesthetic differentials compared to traditional plastic may become amplified as more community members engage in discussions. Furthermore, in close-knit communities where adherence to traditional rules are valued, the pressure to align with prevailing views can deter individuals from adopting innovations like bioplastic bottles, particularly if these products are viewed as unconventional or untested. Given these insights, it becomes clear that increasing discussions or visibility of bioplastic bottles alone is insufficient to guarantee higher adoption rates. Instead, the findings underscore the importance of strategic community engagement and targeted communication efforts. Engaging with community leaders who are viewed as credible and trustworthy can help to reframe the narrative around bioplastic bottles in a more positive light. Additionally, targeted educational events that clearly demonstrate the environmental and practical benefits of bioplastic bottles could mitigate negative perceptions and equip consumers with factual information to counteract prevailing skepticism. Marketing strategies should also be carefully designed to respect local contexts, perhaps starting with smaller, community-based initiatives that allow for direct interaction with the product and gradual building of trust. Implementing continuous feedback mechanisms to monitor community sentiment and adjust strategies accordingly can further enhance the effectiveness of these efforts, ensuring that they remain responsive to the community's evolving perceptions and needs. Through a comprehensive understanding of the complex role of social influences on product adoption, companies and policymakers can more effectively design and implement initiatives that not only increase the visibility of sustainable products like bioplastic water bottles but also positively influence consumer behavior and community norms. This approach promises not only to increase adoption rates but also to raise a more sustainable and environmentally conscious community spirits.

In the context of ABM related to the adoption of bioplastic water bottles, emergent behaviors are those patterns or outcomes that arise from the complex interactions of individual agents, which might not have been predictable from simply analyzing the individual components or rules governing the system. Before employing ABM to study the adoption of bioplastic water bottles, researchers might hypothesize the occurrence of adoption waves based on patterns observed in other eco-friendly products. Historical data and market studies often indicate that consumer adoption of such products can exhibit wave-like or burst patterns (Geroski, 2000). These patterns suggest that once a product surpasses a certain threshold of visibility or credibility among consumers, its adoption rate can accelerate dramatically (Peres et al., 2010). This phenomenon is largely driven by increased consumer confidence and social validation, where prospective users feel reassured by the growing number of adopters and thus are more willing to try the product themselves (Bhattacherjee, 2001). This concept of adoption waves is particularly relevant to bioplastic water bottles, which align closely with growing consumer trends towards sustainability (Young et al., 2010). For example, consider the scenario where a major city implements a successful recycling program and begins promoting bioplastic alternatives as part of an environmental initiative. As more individuals observe bioplastic bottles being used around them, especially by influencers they trust, the visibility of these products increases, enhancing their credibility (Kim and Kim, 2022). This could lead to a significant uptick in adoption as consumers who were previously hesitant but feel more confident now in the product's environmental claims and practical utility (Laroche et al., 2001). A wave of adoption might be further fueled by positive media coverage or endorsements from environmental groups, which extend the perception of bioplastics as a trendy and responsible choice (Hartmann and ApaolazaIbáñez, 2012).

In addition, researchers can reasonably anticipate that misinformation might significantly impede this process. Misconceptions about bioplastics are not uncommon, and these can form substantial barriers to consumer acceptance. For instance, some consumers might hold the mistaken belief that bioplastics degrade too quickly for practical use, lack the durability of traditional plastics, or that they don't offer significant environmental benefits. Myths can create doubts and hesitations among potential users who might otherwise be interested in sustainable alternatives. The effects of misinformation have been well-documented across various product categories and industries (Lewandowsky et al., 2017). In the context of bioplastics, if a significant portion of the market is influenced by incorrect information that questions the product's utility or environmental impact, it could lead to widespread resistance. This resistance can be particularly rooted if influential figures or media outlets broadcast these misconceptions (Boin et al., 2009). To counteract these challenges, a prioritized strategy involving education and clear communication is essential. Educating the public through transparent, accessible information that addresses common myths and explains the benefits and limitations of bioplastics in a factual manner could help mitigate the impact of misinformation. This approach should ideally involve stakeholders from various sectors, including environmental organizations, product manufacturers, and policymakers. By presenting unified, evidence-based messaging, it is possible to gradually shift public perceptions and increase openness to adopting bioplastics. Additionally, showcasing real-world examples of successful bioplastic implementations can serve as a powerful method to illustrate their practicality and environmental advantages, further dispelling prevalent myths and encouraging informed decision-making among consumers (Scheufele and Krause, 2019).

In this study, we only consider a 5 year period based on the weekly decision timeline in the early stage. However, in the long-term prediction, one might predict that the market might reach a saturation point where further adoption slows down significantly. This slowdown typically occurs because the pool of potential early adopters and innovators, who are generally more receptive to new products and ideas, becomes largely exhausted. These individuals are often driven by a desire to be at the forefront of trends or to accept new technologies for their perceived benefits, such as environmental conservation in the case of bioplastics. Once this group is saturated, the challenge then becomes how to appeal to more mainstream consumers and the late adopters, who may be more skeptical. These segments of the market often require different marketing strategies and more convincing to adopt new products. They may not have the same level of enthusiasm or may require more evidence of the practical benefits and costeffectiveness of the products before making a switch. In the context of bioplastics, reaching these consumers could involve emphasizing not just the environmental benefits but also the economic advantages, such as long-term cost savings and durability that matches or exceeds traditional plastics.

Furthermore, this study does not consider the demographics that may impact the adoption rate. Social clustering of behaviors is a well-observed phenomenon, particularly when it comes to the adoption of new technologies and environmentally friendly products. Demographic and social network analyses often reveal that certain behaviors tend to be more prevalent within specific groups, influenced by various factors including age, location, socio-economic status, and cultural background. This clustering effect can be particularly evident in the adoption patterns of innovative products like bioplastics. For instance, urban, younger populations are often quicker to embrace new technologies and sustainable products compared to their rural, older counterparts. This difference can largely be attributed to several factors. Younger individuals in urban areas are typically more exposed to current trends in sustainability and environmental responsibility, both through education and media exposure, as well as through direct interaction in culturally diverse and densely populated urban settings. These settings often provide a fertile ground for the spread of innovative ideas and products, supported by a social infrastructure that values and promotes modernity and environmental consciousness. Additionally, urban areas frequently have better access to the latest products and technologies, accompanied by more targeted marketing campaigns that are often designed to appeal to a younger, more techexperienced demographic. This exposure and accessibility facilitate faster adoption rates among these groups. In contrast, rural and older demographic groups might not only have less access to such products but also tend to have more established habits and preferences which can act as barriers to the adoption of new technologies. Their social networks might also be less influenced by rapid changes in consumer trends, leading to slower adoption rates. Understanding these social clustering effects is crucial for companies and policymakers when planning the launch and marketing strategies for new products like bioplastic water bottles. Using appropriate approaches to fit the specific characteristics and preferences of different demographic groups can significantly enhance the effectiveness of these initiatives. For example, events aimed at younger and urban residents might focus on digital marketing and leverage social media influencers, while efforts to reach older and rural populations could involve more traditional media channels and emphasize practical benefits and ease of transition to new products. Recognizing and addressing the unique dynamics within these clusters can help in effectively spreading new sustainable technologies and behaviors across a broader spectrum of the population.

Given the findings from the ABM study on the adoption of single-use CO_2-based bioplastic water bottles, several strategic recommendations can be made to policymakers, large companies, and other stakeholders involved in the production, distribution, and policy regulation of plastic products. These recommendations aim to enhance the adoption rates of bioplastics and ensure that the transition from conventional plastics is both effective and sustainable. Policymakers play a pivotal role in shaping the market for bioplastics through the strategic use of incentive programs. By making bioplastics more economically attractive, they can catalyze a shift away from conventional plastics, which are often cheaper to produce due to established supply chains and economies of scale. Implementing subsidies, tax incentives, or grants can significantly reduce the production costs associated with bioplastic bottles. This reduction in cost not only makes bioplastics more competitive in the market but also encourages manufacturers to invest in and scale up bioplastic production technologies. For consumers, the cost of switching to sustainable options like bioplastics can be a significant barrier. To address this, policymakers can introduce rebates or offer reduced tax rates on bioplastic products. Financial incentives make bioplastics more accessible to a broader range of consumers by lowering the price point at the point of purchase. This, in turn, can help cultivate consumer habits around sustainability and increase the overall market demand for bioplastics. Additionally, these incentive programs could be designed to be dynamic, scaling up as the technology develops and scaling back as bioplastics become more self-sustaining in the market. By carefully balancing these incentives, governments can effectively support the initial growth of the bioplastic market without long-term dependency on subsidies. This approach not only supports environmental goals but also stimulates economic activity in new and emerging sectors of the green economy.

Strengthening the recycling infrastructure for bioplastics is essential to maximize their environmental benefits and ensure their successful integration into the circular economy. Effective recycling of bioplastics requires specific technologies and processes that can handle biodegradable and compostable materials. Investment in these specialized recycling facilities is crucial, as it enables the proper breakdown and reuse of bioplastic materials, which differ chemically from traditional plastics. This investment not only supports waste reduction but also promotes a sustainable lifecycle for bioplastic products. Additionally, clear labeling is a vital component of a robust recycling infrastructure for bioplastics. Many consumers and waste management facilities currently face confusion over the disposal of bioplastics due to their similarity in appearance to conventional plastics. Implementing standardized labeling that clearly identifies bioplastics as biodegradable or compostable can help alleviate this confusion. This clarity allows consumers to make informed decisions about disposal and ensures that bioplastics are directed towards the appropriate recycling pathways, rather than contaminating the recycling streams of traditional plastics. These steps not only improve the efficiency of recycling programs but also encourage the environmental credibility of bioplastics. When consumers see that bioplastic products are not only sourced sustainably but also managed responsibly at the end of their lifecycle, it enhances their trust and confidence in these products as truly eco-friendly alternatives. This trust can drive higher adoption rates and broader acceptance of bioplastics in the market. By investing and regulating in advanced recycling facilities and clear labeling, policymakers and industry leaders can significantly impact the sustainability and public perception of bioplastic products.

To further promote the adoption and integrity of bioplastic usage, the implementation of regulations and clear standards is significant. By introducing regulations that require a minimum content of bioplastics in certain products or packaging types, governments can create a baseline requirement that ensures a steady demand for bioplastics, thus encouraging industries to innovate and scale up their bioplastic production capabilities. This approach reflects successful strategies employed in other sectors, such as renewable energy, where similar indicate have significantly promoted industry growth and technological advancement. In addition to setting usage requirements, it is equally important to establish clear standards defining what qualifies as a bioplastic. This is importance for preventing greenwashing, a practice where products are lyingly marketed as environmentally friendly, even when their production or life cycle impacts are questionable. Clear standards will help consumers make informed choices, ensuring that the products they purchase actually offer reduced environmental impacts. These standards should specify criteria such as the source of the materials, the production process, the biodegradability, and the compostability of the bioplastic products. Such regulatory frameworks and standards not only support environmental objectives but also build consumer trust in bioplastic products. When consumers are confident that the bioplastics they are buying meet strict environmental standards, their willingness to choose bioplastics over conventional plastics increases. This trust, supported by a transparent and reliable regulatory environment, can drive the wider adoption of bioplastics, contributing to a reduction in plastic waste and fostering a more sustainable economy.

To ensure the effectiveness and relevance of policies aimed at promoting bioplastics, it is crucial to establish robust mechanisms for monitoring and adapting these policies. This adaptive management approach involves continuous assessment of both the outcomes of existing policies and the market's response to bioplastics. By keeping a close watch on these dynamics, policymakers can gather valuable data that highlights the successes and shortcomings of current measures. The process should include regular evaluations of how well the policies are meeting their intended environmental and economic objectives. This could be achieved through collecting and analyzing data on bioplastic production volumes, usage rates in various sectors, consumer acceptance levels, and the environmental impact relative to conventional plastics. Additionally, feedback from industry stakeholders, environmental groups, and consumers can provide insightful perspectives on the practical challenges and opportunities presented by these policies. Based on the insights gained from these evaluations, policies may need to be refined or recalibrated. For instance, if bioplastic adoption rates are not meeting targets, it may be necessary to adjust incentive structures or strengthen educational campaigns. Conversely, if certain types of bioplastics are performing well and exceeding expectations, policies could be modified to further encourage their use, perhaps by expanding instructions or increasing subsidies. This approach not only ensures that bioplastic policies remain aligned with evolving market conditions and technological advancements but also helps to maintain their effectiveness and public support over time. By adapting to new information and changing circumstances, policymakers can sustainably integrate bioplastics into the economy, thereby contributing to broader environmental goals and fostering innovation in green technologies.

Engaging community leaders and social influencers is a critical strategy for promoting the adoption of bioplastics. The influence of respected and well-known figures within communities can have a profound impact on public perception and behavior. As highlighted by this study, social influence significantly affects adoption rates. Companies and policymakers should collaborate with these leaders and influencers to utilize their reach and credibility. This can involve organizing community events, initiating social media pathways, and other outreach efforts that feature endorsements from these key figures. For instance, local community leaders can be invited to participate in workshops and seminars about the benefits of bioplastics, where they can share their positive experiences and insights directly with the community. Similarly, social media influencers who are known for their commitment to sustainability can help communicate the environmental advantages of bioplastics to a broader audience. Furthermore, involving these leaders in the policymaking process can ensure that the strategies developed are culturally and socially relevant, enhancing their effectiveness. By working closely with community figures, companies and policymakers can create a more engaging and persuasive narrative around bioplastics, which is essential for shifting public attitudes and encouraging widespread adoption. This approach not only participates into the social networks of these influencers but also utilizes their ability to shape opinions and lead community-wide changes in consumer behavior.

By adopting these recommendations, decision-makers can significantly influence the market dynamics for bioplastics, enhancing their adoption and contributing to broader environmental sustainability goals. These strategies highlight the importance of an integrated approach that combines economic incentives, educational efforts, regulatory frameworks, and community engagement to transition away from conventional plastics effectively.

2. Environmental, human health, and CO_2 payback estimation and comparison of enhanced weathering for carbon capture using wollastonite

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Danyi Feng: Designed Research, Performed Research, Analyzed Data, Wrote the Paper.

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2.1. Abstract

Negative emission technologies (NETs) are emerging pathways to remove carbon dioxide (CO_2) from the atmosphere in order to achieve the target of the 2015 Paris Agreement that restricts global temperature increases between 1.5 ◦C and 2 ◦C. In recent years, enhanced weathering

(EW) has drawn considerable attention as a potential carbon dioxide removal technology (CRD). The advantages of EW are not only to capture CO_2 but also to improve the productivity of agricultural land and intensify soil water retention. Here, a comprehensive literature review is conducted to inform a cradle-to-grave life cycle impact assessment of EW of wollastonite. While previous studies report that the transportation process has the greatest environmental and human health impacts where natural rocks are used, there is currently a gap in the literature with respect to the implications of synthesized rocks. The aim of this work is to analyze and compare the environmental, human health, and CO_2 payback period performances of EW for carbon capture using synthetic and natural wollastonite. The functional unit is 1 kg CO_2 removed. The results indicate that the natural scenario performs better from environmental, human health, and CO_2 payback perspectives when compared to the synthetic scenario.

2.2. Introduction

Since 2000, the global carbon dioxide (CO_2) levels in the atmosphere have increased by approximately 93 Gt CO_2, a 12% increase (Lindsey, 2021). However, as the pandemic in 2020 affected the global economy and human activities, the average annual global fossil CO_2 emission presented a downtrend with 6% (34.5 Gt CO_2) fossil CO_2 emission decline compared to 2019: the United States decreased emissions by 9.9% and only China increased emissions by 1.5% (European Commission et al., 2021; Terlouw et al., 2021). This reduction although temporary, illustrates the potential for changes in human behavior to impact emissions. Immediate actions are required to achieve the goal of the 2015 Paris Agreement that limits global temperature increases between 1.5 ℃ to 2 ℃ (IPCC, 2015; Terlouw et al., 2021). Deployment of negative emission technologies (NETs) is needed to remove CO_2 in order to restrict the increasing carbon emission level to reach climate stabilization in the future as emphasized by Intergovernmental Panel for Climate Change (IPCC) (Goll et al., 2021b; McQueen et al., 2020). There are seven major classes of NETs, including carbon capture and storage with bioenergy, direct air capture, enhanced weathering, reforestation and afforestation (Li and Wright, 2020), biological or chemical carbon sequestration by the ocean, agricultural practices, and biochar (Smith, 2016; Smith et al., 2016). Additionally, the most recent literature indicates that other new concepts of carbon removal technologies are being developed, which can be divided into CO_2 capture technologies (e.g., chemical looping combustion capture), CO_2 utilization technologies (e.g.,beverage carbonation), and CO_2 storage technologies (e.g., storage in basalt and ultramafic rocks via carbon mineralization) (Hong, 2022). Enhanced weathering (EW) is a potentially essential technology for carbon dioxide removal (CDR) that has attracted a growing amount of attention in recent years (Lefebvre et al., 2019). However, the question still exists as to its environmental impacts and sustainability considerations.

Since the 1990s, using the natural weathering process of silicate rocks has been suggested as a substitute approach for capturing CO_2 (SEIFRITZ, 1990) and initially studied in detailed for industrial application (Lackner et al., 1995b). Weathering is divided into physical, chemical, and biological processes due to the aggregated action of microbes, water, and air on rock breakdown and crystallization (Ribeiro et al., 2020). For chemical processes, EW works on the principle of utilizing disintegrated silicate minerals (e.g., wollastonite, olivine) (Bach et al., 2019) to sequester CO_2 from the atmosphere, and then transporting and permanently storing the final dissolved products (e.g., $CaCO_3$) in a deep layer in an ocean (Hartmann et al., 2013; Strefler et al., 2018). Two chemical reactions have been commonly used to represent the process of EW: (1) extract cation ions (e.g., Ca^{2+}, Mg^{2+}) from decomposed minerals and react with CO_2 and water to release bicarbonate ions, commonly using wollastonite rocks ($CaSiO_3$) (Equation (1)) (Kakizawa et al., 2001; Rinder and von Hagke, 2021).

$$CaSiO_3 + 2CO_2 + 2H_2O \rightarrow Ca^{2+} + 2HCO_3^- + SiO_2 + H_2O \qquad \text{Equation 3}$$

(2) form the precipitation of solid carbonates by reaction between cation ions and bicarbonate ions (Equation (2)) (Lefebvre et al., 2019).

$$Ca^{2+} + 2HCO_3^- \leftrightarrow CaCO_3 \downarrow + CO_2 + H_2O \qquad \text{Equation 4}$$

The global carbon cycle is impacted by EW due to the elevated uptake of atmospheric CO_2 (Zapata-Rios et al., 2015). The potential effectiveness of EW in CO_2 removal is 5% to 15% (Beerling et al., 2020), approximately 0.4 to 2 Gt CO_2/year (Goglio et al., 2020; Lal, 2004). It emphasized that EW could reduce 30-300 ppm CO_2 (2.9-8.5 Gt CO_2/year) levels in the atmosphere until 2100 (Tan and Aviso, 2021; Taylor et al., 2016). Besides, EW applied in agricultural land has a high potential to reduce the nutrient runoff (De Oliveira Garcia et al., 2020), improve the productivity (Liang et al., 2021), and enhance soil water retention (Beerling et al., 2020). Nevertheless, the capacity of EW for carbon capture depends on the application area, type of rock selected, silicate composition, the particle size of the rock (Renforth, 2012), application rate (Lefebvre et al., 2019), and comminution technique (Moosdorf et al., 2014). Table 1 summarizes the CDR rate related to the type of rocks, landcover variety, and climate features from previous case studies.

Table 1. Summary of reviewed case studies.

Reference	Type of rocks	CO_2 removal rate (Gt CO_2/year)	Landcover	Climate
(Hartmann and Kempe, 2008)	Basalt	1.8	Cropland	Tropical wet and temperate wet
(Renforth et al., 2011)	Silicate mineral	0.7 – 1.2	–	–
(Strefler et al., 2018)[a]	Dunite	95	Cropland	Global
(Strefler et al., 2018)[b]	Basalt	4.9	Cropland	Global
(Lefebvre et al., 2019)	Powdered Basalt	0.0013 – 0.0024	Cropland	Tropics (Brazil)
(Goll et al., 2021b)	Powdered Basalt	2.5	Vegetated land	Global
(De Oliveira Garcia et al., 2020b)	Powdered Basalt	44	Forest	Global

In general, basalt dust has a varying removal efficiency that is applied in cropland because of different climate regions. Converting all carbon removal rates on a global scale, EW has the highest effectiveness in a warm and humid areas (Hartmann and Kempe, 2008; Strefler et al., 2018). In contrast with the cropland field, the forest application field has a higher sequestration rate. Strefler et al. (2018) compared two kinds of silicate rocks (basalt and dunite), and the result found that dunite has a higher removal rate than basalt due to higher sufficient carbon sequestration potential. The silicate minerals for carbon capture in Renforth et al. (2011) are extracted from waste, including aggregate and mine waste, construction and demolition waste, iron, and steel waste, etc., and the CO_2 removal range is between 1.9 to 3.2 Gt CO_2 per year. For example, Zhang et al., (2023) and Jia et al., (2022) utilized non-hazardous industrial wastes, which included desulfurization gypsum, coal fly ash, tailing, steel slag, and refining slag, to sequestrate CO_2 in Shandong province, China. The estimation from this study is that approximately 306 Mt CO_2 will be fixated by non-hazardous industrial waste in Shandong Province, China from 2020 to 2030 (around 12.73 Mt CO_2-13.77 Mt CO_2 per year). Moreover, the carbonation efficiency of silicate minerals from waste is 10% to 60% higher than untreated natural silicate resources (Renforth, 2019). However, Renforth (2019) did not consider the application field and climate for EW. In these studies, the methodologies employed in EW carbon capture capability estimate are varied, likely due to the relatively nascent nature of their area of study, and some of them considered the environmental consequences of EW.

In this paper, a literature review is presented based on current studies regarding the LCA of EW for carbon capture. The goal of this paper is to recognize and address critical research gaps through understanding various environmental and human health impacts associated with variety of silicate rocks, application rate of silicate minerals, transportation distances, and geographic application area.

2.3. Literature Review of LCA

Life cycle assessment (LCA) is a widely used approach for analyzing the environmental and human health implications of a product or system in all life cycle phases, from raw materials extraction, manufacture, use, to disposal or reuse (Hicks et al., 2015a). To date, only Cooper et al. (2022), Eufrasio et al. (2022), Koornneef and Nieuwlaar (2012), and Lefebvre et al. (2019) analyzed various environmental and human health impact categories of EW using LCA. Although there has not been a great deal of LCA studies devoted to EW, there have been quite a few which consider the environmental impacts of rock crushing (Kittipongvises et al., 2016; Pradhan et al., 2019; Rosado et al., 2017) for various construction applications. The current research findings on each life cycle stage of EW in the three studies will be discussed in the following sections.

Raw materials. Both Lefebvre et al (2019) and Eufrasio et al (2022) considered using pulverized basalt rock as raw material. Basalt is a type of fine-grained volcanic rock dark color which is formed from the lava flows (Ercenk et al., 2018; Isnugroho et al., 2018). Approximately 2.5 million km^2 of basalt rocks (Ercenk et al., 2018) are distributed on oceanic islands (e.g. the island of Hawaii, the Faroe islands, the Reunion islands) (Schmincke, 2003) and large igneous provinces (e.g. Deccan Traps in India, the Chilcotin Group in Canada, the Columbia River Plateau in United States) (Philpotts and Ague, 2009). The classification of basalt can be divided into alkali basalt and subalkali basalt based on the state of silica saturation (Le Maitre, 2002). Numerous basalt varieties, including calc-alkali basalt (high-alumina basalt), mid-ocean ridge basalt, tholeiitic basalt, transitional basalt, etc., are included in the subalkali basalt group (Le Maitre, 2002). It is an inexpensive and abundant material that is commonly used in construction (Isnugroho et al., 2018), especially for concrete and asphalt (Tan and Aviso, 2021). By definition, the composition of basalt contains up to 52% SiO_2 (Le Maitre *et al.*, 1989). Furthermore, the application rate of basalt is one of the significant factors to drawdown CO_2 concentration. Three basalt application rates, including 5, 20, and 50 t/ha, were considered in (Lefebvre et al., 2019).

Besides, basalt has the same chemical and mineralogical composition as dolerite, diabase, and gabbro but has different grain sizes due to different crystallization histories, including volcanic, shallow intrusion, and deep intrusion, respectively (Brooks, 2022).
Therefore, as long as the particles are crushed down to the same particle size, the EW behavior for these rocks will be same.

Koornneef and Nieuwlaar (2012) and Cooper et al. (2022) selected olivine as an option of raw material. Olivine is a common silicate mineral in Earth's subsurface (Flipkens et al., 2021) that derived from mantle magmas (Qi et al., 2021; Yao et al., 2021) with 92% forsterite and 8% fayalite as representative composition of a natural olivine solid solution (Kersbergen, 2020). There are four main types of olivine, including Mg-rich olivine, forsterite (Mg_2SiO_4), Fe-rich olivine, and fayalite (Fe_2SiO_4) (Qi et al., 2021). Compared to basalt, olivine is more effective (Edwards et al., 2017). However, the proportion of Fe in olivine (Kersbergen, 2020), temperature (Schuiling and Krijgsman, 2006), and precipitation volume (Schuiling, 2012) are significant features can affect weathering efficiency. Olivine is one of the rock-forming mineral that help to maintain a stable CO_2 condition in the atmosphere in its natural state (Kersbergen, 2020).

Manufacture. Rock extraction and comminution are two priority manufacturing processes (Cooper et al., 2022; Eufrasio et al., 2022; Koornneef and Nieuwlaar, 2012; Lefebvre et al., 2019). Drilling to embed explosives in quarries is the first step of rock extraction (Rosado et al., 2017). After mining, the rocks are loaded into trucks and transported to the comminution facilities for crushing and grinding (Rosado et al., 2017). The purpose of comminution is to obtain the smallest feasible particle size of rocks in order to achieve satisfactory weathering rates (Koornneef and Nieuwlaar, 2012; Rinder and von Hagke, 2021). The particle size used in Koornneef and Nieuwlaar (2012) and Lefebvre et al. (2019) for EW are 75 μm and less than 5 mm, respectively. When the particle size is smaller, there is more rock powder dissolved and able to react with CO_2 (Rinder and von Hagke, 2021). Moreover, crushing and grinding is an energy intensive process (Koornneef and Nieuwlaar, 2012). Therefore, the energy requirement for comminution is one of the important parameters to consider when selecting machinery as well as crushing rate, reduction ratios, and size acceptance (Koornneef and Nieuwlaar, 2012; Lefebvre et al., 2019). Eufrasio et al. (2022) analyzed two future energy scenarios (Business-As-Usual (BAU) and 2℃) for EW deployment in 12 countries, including Italy, France, Germany, Spain, India, Poland, Mexico, China, United States, Brazil, Indonesia, and Canada. BAU scenario is based on current policies that countries continue to use fossil fuels for energy generation, and the 2℃ scenario is to aim Paris Agreement objective with 66% probability (Eufrasio et al., 2022). For transportation consideration, trucks are one of the main transportation options utilized to carry out rocks from quarries (Eufrasio et al., 2022), crushing and grinding facilities (Cooper et al., 2022), and to the spreading field (Koornneef and Nieuwlaar, 2012; Lefebvre et al., 2019). Besides, rail transportation is selected when the distance between the mining area and the spreading field is long (Eufrasio et al., 2022). Another option of transportation is via ship if the spreading field is near the seacoast (Koornneef and Nieuwlaar, 2012).

Use phase. Deployment of crushed silicate rock as fertilizer applied in agricultural land (Barão and Teixeira, 2016; Kantola et al., 2017) to improve nutrient uptake availability by plants (Liang et al., 2021; Ribeiro et al., 2020) has already been employed in recent decades. To date, one LCA study has analyzed the environmental impacts of two different rock fertilizer types. Barão and Teixeira (2016) performed a comparison of production and application of silicate fertilizer and phosphorus fertilizer using LCA. Sodium silicate (Na_2SiO_3) and calcium silicate (Ca_2SiO_4) are most the often used silicate fertilizers in four silicate accumulator crops which are sugarcane, sugar beet, wheat, and barley. In this study, 12 ton/year of sodium silicate was assumed as raw material with 64 ton/year of lime and 14 ton/year of hydrochloric acid to produce 69 ton/year of calcium silicate fertilizer. Therefore, the main consideration in use phase is spreading and utilizing minerals on cropland to remove CO_2. Besides, enhancements to farm soil quality may potentially reduce the demand for synthetic fertilizers, which resulting in lower carbon footprint. However, it is an outside scope of this study.

End of life. Losses for silicate mineral resources are considered as dissipative flows. The definition of dissipation is that the movement of resources into the environment (Beylot et al., 2021, 2020; Owsianiak et al., 2021) or disposal facilities is irreversible or irrecoverable through technologies and economics (Beylot et al., 2021, 2020; Charpentier Poncelet et al., 2021; Owsianiak et al., 2021; Zimmermann and Gößling-Reisemann, 2013). For EW, the silicate resources and products (e.g., $CaCO_3$) have been discarded and distributed to the environment (e.g., groundwater, ocean) during the use phase. Therefore, the dissipative flow of silicate resources could be included in end of life phase. Currently, however, no study has analyzed the environmental and human health impacts of dissipation for silicate rocks on EW.

2.4. Overall LCA

Previous LCA studies. To date, there are four LCA studies to analyze various environmental and human health impacts of EW that are applied on croplands for carbon capture. Lefebvre et al. (2019) reported seven environmental and human health categories via the CML impact assessment method, involving cumulative energy demand (CED), greenhouse gas (GHG) balance, abiotic depletion, acidification, freshwater ecotoxicity, human toxicity (carcinogenic and non-carcinogenic). They concluded that the transportation has the maximum contribution of all seven impacts. Additionally, based on three (5, 20, 50 ton/ha) application rates of powdered basalt rock, the highest application rate can sequester most CO_2 in São Paulo State, Brazil. Furthermore, Koornneef and Nieuwlaar (2012) analyzed nine environmental and human health impacts categories through the CML 2 baseline 2000 method. The main contributor is transportation for all environmental impacts, which is consistent with (Lefebvre et al., 2019) study. In addition, the electricity for crushing and grinding is another dominant process for ecotoxicity categories. However, the remaining processes have negative climate change impact compared to the four main manufacturing processes, which means the concentration of CO_2 sequestered is larger than the concentration of CO_2 emitted. Making this a viable technology to consider for carbon capture. Eufrasio et al. (2022) used ReCiPe (H) method to weight 18 midpoint impacts indicators into 3 endpoint indicators depends on 12 nations' energy mix, including resource depletion (fossil fuel depletion), ecosystem loss (natural land transformation potential, land occupation, acidification, eutrophication, ecotoxicity of water, and global warming potential), and human health impacts (human toxicity, photochemical oxidant formation, and ozone depletion). They reported that comminution processes and transportation are two dominant contributors to all environmental and human health impacts for all 12 nations, including China, India, United States, Brazil, Canada, Indonesia, Mexico, France, Germany, Spain, Portland, and Italy. This is because high energy and fuel are required in rock comminution and transportation. Cooper et al. (2022) compared 17 environmental and human health impacts of 5 NETs (afforestation/reforestation, EW, mangrove restoration, bioenergy with carbon capture and storage, and direct air capture) via IPCC AR and ReCiPe methods, including CO2 equivalence, air (photochemical ozone formation and stratospheric ozone depletion), freshwater (consumption, ecotoxicity and eutrophication), marine environments (marine ecotoxicity and eutrophication), human health (human toxicity, cancer and non-cancer), resources and land (terrestrial acidification and ecotoxicity, land use and metal depletion). Depending on the results, EW has higher impacts to freshwater, marine environment, and human health, but lower in other implications. Cooper et al. (2022) reported that grinding, transportation, and spreading contributes the most to environmental and human health implications. These findings supported the results from Lefebvre et al. (2019) study. Furthermore, mining process is a majority in natural land transformation and land occupation potential for all 12 nations.

Cost. Beerling et al. (2020) determined the CO_2 removal cost via EW with croplands by using a techno-economic approach. The results demonstrated that if four countries (China, India, United States, and Brazil) deploy EW on agricultural land, they have the potential to contribute 0.5 – 2 Gt CO_2/year reduction with sequestration cost around \$80 – \$180/ton CO_2. Strefler et al. (2018) compared the potential carbon removal rate and costs of both dunite and basalt rocks for EW through techno-economic assessment as well. The removal efficiency of dunite and basalt applied in cropland is 95 Gt CO_2/acre and 4.9 Gt CO_2/acre with capture costs \$60/ton CO_2 and \$200/ton CO_2, respectively. McQueen et al. (2020) estimated net removed cost is between

\$46/ton CO_2 to \$159/ton CO_2 for EW. McLaren (2012) summarized that using available olivine in this world to sequester 1 Gt CO_2/year will cost \$20 - \$40/ton CO_2. The carbon capturing costs vary for EW due to the different rock types selected, differences in the methods of processing, and distance to transport.

2.5. Summary of Current Research Gaps

Several research gaps exist in the life cycle considerations for silicate rock sequestration of EW. First, only one comprehensive LCA study of EW was found, hence the LCA has the potential to be skewed based on the lack of variability of studies. Second, all of the papers discussed the crushed basalt and olivine rocks, no research study analyzes the synthesized pulverized wollastonite rocks for environmental implications of EW. Synthetic silicate minerals may have higher reactive efficiency than natural minerals (Bodor et al., 2013; Haque et al., 2020a). Moreover, the silicate manufacturing processes could be used with other technologies (e.g., geological sequestration, cement production) to reduce the overall environmental impacts (Caserini et al., 2019; Litynski and Damiani, 2013).

2.6. Methods

2.6.1. Goal and scope

The purpose of this work is to quantify and compare the environmental and human health implications of EW for carbon capture using synthetic and natural wollastonite. The functional unit (FU) is 1 kg of CO_2 removed. There is no life span considered in this study because it is assumed that the wollastonite is a single-use rock, regardless of whether it is synthetic or natural.

A system boundary includes raw material extraction, manufacture, transportation, use, and endof-life phases, as presented in Figure 1. It is anticipated that the synthetic wollastonite will have a greater environmental impact due to the additional necessitated processing when compared to natural wollastonite. However, the question exists as to whether the increased environmental impact will shift the carbon balance, negating the anticipated carbon negative benefits.

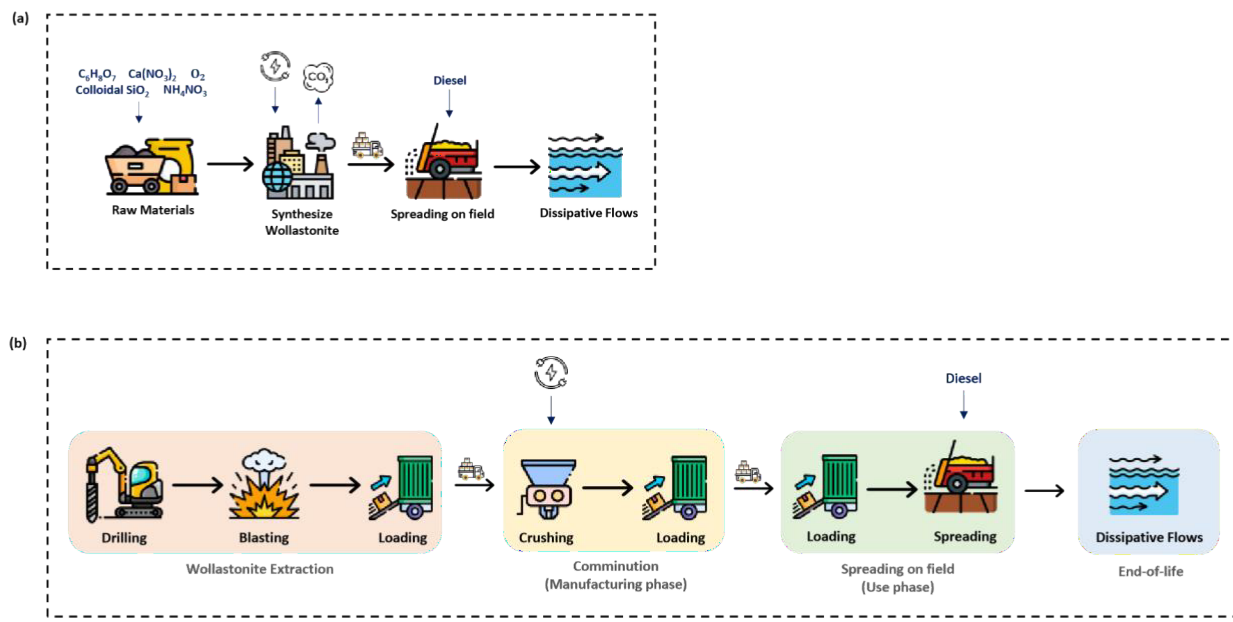

Figure 6. System boundary of a) synthetic wollastonite, and b) natural wollastonite.

2.6.2. Natural wollastonite

Lefebvre et al. (2019) summarized the process stages (rock extraction, comminution, transportation, and spreading) and inventories of each life cycle stage to sequester CO_2 from the air that used natural rocks, as shown in Table A1. The stoichiometry is used to estimate the quantity of CO_2 removed when 1 kg wollastonite reacted based on the Equation 3. Therefore, the removal efficiency of wollastonite to sequester CO_2 is 0.38 kg CO_2 per kg of wollastonite applied. The wollastonite extraction phase contains drilling, blasting, loading, and transportation to the manufacturing phase. The production capacity of wollastonite quarried in the United States is 29,880 kg/hour (Nair and Sairam, 2021). Inserting explosives for drilling is the first step in the rock extraction process (Rosado et al., 2017). A front loader is used to load shattered wollastonite in a truck and transport it to a comminution facility that is 1 km away from the quarry (Lefebvre et al., 2019). The electricity that is used to crush wollastonite to reach 5 mm particle size is the only consideration in the comminution stage (Lefebvre et al., 2019). After comminution, the crushed wollastonite is loaded in a truck and transported to the spreading field that is modeled to be 65 km away from the processing facility, based on the assumptions of Lefebvre et al. (2019). Transportation of pulverized wollastonite from the quarries to the comminution facility, and then from the crushing facility to the spreading field are considerations in this study. After wollastonite is delivered to the field, a front loader is used to load rock into a conventional lime spreader which was assumed to be a field spreader in this study, and only the diesel consumption for the wollastonite spreading is calculated based on the agricultural machinery consumption (Lefebvre et al., 2019). In the end-of-life phase, calcium carbonate ($CaCO_3$) and silicon dioxide (SiO_2) are considered as dissipative flows.

2.6.3. Synthetic wollastonite

A detailed inventory of synthetic wollastonite can be found in Table A2. All inputs and outputs for wollastonite synthesis are from Huang and Chang (2009). The CO_2 removal rate is assumed to be the same as natural wollastonite by using stoichiometry according to Equation 3, which is 0.38 kg CO_2 removed by 1 kg wollastonite applied. Four chemicals are used as raw materials in this scenario, including calcium nitrate ($Ca(NO_3)_2$), colloidal silicon dioxide (SiO_2), ammonium nitrate (NH_4NO_3), and citric acid ($C_6H_8O_7$), and all reagents have the highest purity to avoid further purification. Firstly, dissolve $Ca(NO_3)_2$, NH_4NO_3, and $C_6H_8O_7$ in deionized water, and add colloidal SiO_2 to this solution under constant stirring. This solution is then dehydrated and heated in order to remove water to form a sticky gel. After the water is fully evaporated, the temperature is increased to combust viscous gel to transform the gel phase into solid particles. The outputs in this reaction not only produce wollastonite powder, but also produce and emit carbon dioxide (CO_2), nitrogen gas (N_2), and water (H_2O). The overall chemical reaction during combustion is shown below:

$$Ca(NO_3) + 2C_6H_8O_7 + 7NH_4NO_3 + 3O_2 + SiO_2 \rightarrow CaSiO_3 + 12\ CO_2 + 8N_2 + 22H_2O$$

The amount of chemicals as inputs and outputs to produce 1 kg wollastonite are calculated by using stoichiometry. The production rate to yield wollastonite powder in this experiment is 60%, which is a significant factor to calculate the quantity of raw materials needed in synthetic processes. In this study, 60%, 80%, and 99% yield rates of mass are assumed to acquire 1 kg wollastonite, in order to account for potential future maturity of the synthesis processes. For the manufacturing stage, the amount of electricity usage for dehydrating, heating, and combustion is not provided in Huang and Chang (2009). However, Piccinno et al. (2016) and Parvatker et al. (2019) demonstrated the steps to calculate energy and electricity demand in industrial scale chemical processes. The calculations from Piccinno et al. (2016) and Parvatker et al. (2019) are used to estimate the amount of electricity that produce 1000 kg wollastonite, and we converted quantity of electricity to 1 kg scale. The truck is considered to transport rock to the spreading land, and the average transportation distance is assumed to be 65 km based on assumptions by Lefebvre et al. (2019). After the wollastonite is delivered to the spreading field, a conventional lime spreader is assumed to be used, and only diesel consumption is calculated for the spreading of material (Lefebvre et al., 2019). With the natural wollastonite scenario, the dissipative flows are considered in the end-of-life phase, including $CaCO_3$ and SiO_2. The amounts of dissipative flows released are estimated using the same method as in the natural wollastonite scenario.

2.6.4. Life cycle environmental and human health assessment

Ecoinvent and USLCI inventories, and the TRACI (version 2.1) method are used to analyze the environmental and human health impacts with SimaPro software (version 9.2.0). Ten midpoint categories are considered, including seven environmental impacts (ozone depletion (OD, kg CFC-11 eq), global warming potential (GWP, kg CO_2 eq), smog (SM, kg O_3 eq), acidification (AC, kg SO_2 eq), eutrophication (EU, kg N eq), ecotoxicity (ET, CTUe), and fossil fuel depletion (FFD, MJ surplus)), and three human health indicators (carcinogenic (HHc, CTUh), noncarcinogenic (HHnc, CTUh), and respiratory effects (RE, kg PM2.5 eq)) (Feng et al., 2021; Hicks et al., 2015a). The TRACI method is a midpoint approach which is developed by U.S. EPA and based on comprehensive and accountable data and models available in the U.S. (Ghamkhar et al., 2022b).

Equation 5 is utilized to calculate environmental and human health impacts (I) and scale to one FU.

$$I = \frac{I^{RM} + I^{M} + I^{S} + I^{DE}}{R_{CO2}} \qquad \text{Equation 5}$$

where, I_{RM} represents the total impact of the raw material phase based on 60% production rate. I_M represents the total impact of the wollastonite synthesis phase. I_S represents the total impact of wollastonite spreading on the application field. I_{DF} represents the total impact of dissipative flows in the end-of-life phase. R_{CO2} is the total amount of CO_2 removed per year which is 0.76 kg for both synthetic wollastonite scenario and natural wollastonite scenario.

2.6.5. Breakeven and sensitivity analysis

Environmental breakeven analysis is a tool to determine the breakeven point of global warming potential, which is also defined as the CO_2 payback period. This is calculated by ensuring that the CO_2 equivalent emissions linked with the raw materials, electricity, transportation, and diesel utilized in the spreading phase equal the amount of CO_2 eliminated by 1 kg of wollastonite for both scenarios. Additionally, the breakeven point of various electricity resources is defined. The relationship between emitted CO_2 and removed CO_2 is represented in Equation 6.

$$Removed\ CO_2 = GWP_{RW} + GWP_{E,U} \times T_E + GWP_{T,U} \times T_T + GWP_{S,U} \times T_S \qquad \text{Equation 6}$$

where, GWP_{RW} is the global warming potential of raw materials which is not changed due to the amount of wollastonite to capture carbon cannot be changed. $GWP_{E,U}$, $GWP_{T,U}$, and $GWP_{S,U}$ are the unit global warming potential of electricity (per kWh), transportation (per kg-km), and diesel for spreading field (per kg), respectively. T_E, T_T, T_S are total amount of electricity, transportation and diesel used for wollastonite synthesis or natural wollastonite application.

A sensitivity analysis was conducted to identify which parameters are sensitive to the LCA results. In this study, various types of electricity resources are used as inputs to examine the influence on all environmental and human health impact outcomes for the two scenarios. The tested electricity generation inputs include grid mix, wind, biomass, coal, oil, photovoltaic (PV), and nuclear. The percentage of yield contains 60%, 80%, and 99% to acquire 1 kg wollastonite. Furthermore, Monte Carlo simulation in SimaPro software was conducted for 1000 runs with 95th confidence interval for each impact category in order to estimate the uncertainty of output parameters.

2.7. Results

2.7.1. Environmental and human health implication comparison of two scenarios

The estimated characterization results of the various production rate for wollastonite synthesis and natural wollastonite under FU are provided in Table 2. For the synthesis scenario, when the production rate from 60% increased to 80%, the environmental and human health implications decreased by 26-34%. If the % yield rate increases from 80% to 99%, 23-26% of environmental and human health impacts are reduced. Improving the production yield rate from 60% to 99% will decrease both environmental and human health performances by 55-68%. Therefore, the production rate is inversely proportional to environmental and human health impacts, which means the higher % yield rate can cause lower implications. On the basis of one FU, shifting 1 kg wollastonite production and usage from natural wollastonite scenario to synthetic wollastonite scenario of 99% production rate will increase environmental and human health impacts by 99.77-

99.96%. The environmental and human health implications of two scenarios follow this trend: 60% production rate > 80% production rate > 99% production rate for wollastonite synthesis > natural wollastonite acquisition. Overall, natural wollastonite has better performance in both environmental and human health perspectives.

Table 2. Impacts comparison of two scenarios considered in this study according to one FU.

Impact categories	**Unit**	**Synthesis scenario**			**Natural scenario**
		60%	80%	99%	
Environmental impacts					
Ozone depletion (OD)	kg CFC-11 eq	1.29×10^{-5}	9.65×10^{-6}	7.80×10^{-6}	6.23×10^{-9}
Global warming (GW)	kg CO_2 eq	107.62	85.75	69.30	0.031
Smog (SM)	kg O_3 eq	5.27	3.96	3.20	0.0074
Acidification (AC)	kg SO_2 eq	0.55	0.41	0.33	2.94×10^{-4}
Eutrophication (EU)	kg N eq	0.32	0.24	0.19	7.20×10^{-5}
Ecotoxicity (ET)	CTUe	752.69	564.55	456.23	0.21
Fossil fuel depletion (FFD)	MJ surplus	82.47	61.87	50.00	0.073
Human health impacts					
Carcinogenic (HHc)	CTUh	4.16×10^{-6}	3.12×10^{-6}	2.52×10^{-6}	1.06×10^{-9}
Non-carcinogenic (HHnc)	CTUh	2.11×10^{-5}	1.58×10^{-5}	1.28×10^{-5}	7.23×10^{-9}
Respiratory effects (RE)	kg PM2.5 eq	0.103	0.077	0.062	3.30×10^{-5}

The contribution of different life cycle inventories associated with the various impact indicators for the synthesis and natural wollastonite scenarios are presented in Fig. 2. For the natural wollastonite scenario (Fig. 4 (a)), the transportation is the dominant contributor which impacts approximately 61%, 48%, 38%, 54%, 65%, 50%, 71%, and 41% of OZ, GW, EU, HHc, HHnc, RE, ET, and FFD, respectively. The higher SM and AC impacts are a result of the higher loading operation from the extraction phase to the use phase. There are no environmental and human health impacts in the end-of-life phase because no bioaccumulation and acute toxicity after $CaCO_3$ and SiO_2 precipitations are emitted into water (Fruijtier-Pölloth, 2012; MTI Environmental Health and Safety Service Department, 2005). For the synthetic wollastonite scenario (Fig. 4 (b)), citric acid for synthesis manufacturing is the significant contributor to all impact indicators from 44.52% for GW to 65.29% for OD. This is due to a large consumption of feedstock and energy used for fermentation in citric acid production (Parsons et al., 2019). The ammonium nitrate and grid mix electricity for wollastonite manufacturing led secondary contribution to total implications.

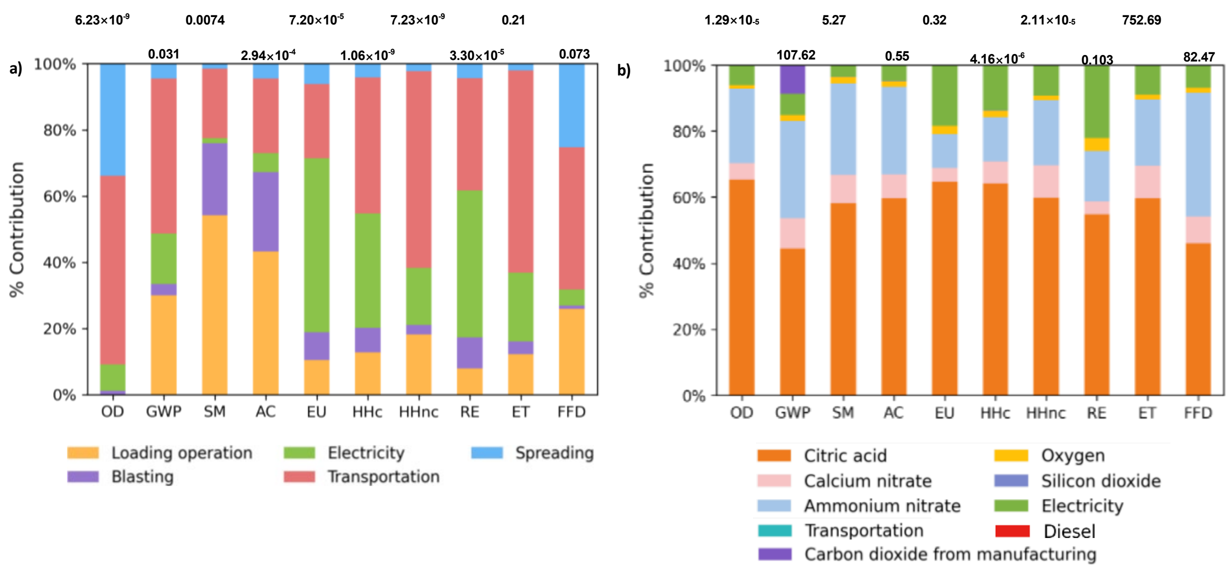

Figure 7. Percentage contributions of different life cycle stages to the environmental and human health impacts under (a) natural wollastonite and (b) synthetic wollastonite scenario.

2.7.2. Breakeven analysis

The breakeven analysis is relevant to determine the relationship between the carbon emissions of each life cycle stage and the total amount of carbon sequestrated. Ten factors are considered, including loading operation, transportation, diesel for rock spreading, and electricity (grid mix, wind, biomass, coal, oil, PV, diesel, and nuclear). The annual natural wollastonite production is assumed to be consistent, and the blasting stage only considered annual wollastonite production, hence in the breakeven analysis for wollastonite blasting is not counted. The results of the natural wollastonite for seven electricity scenarios are shown in Fig. 5. The balance points of loading operation, transportation, and diesel are approximately 0.012 hours, 4493.50 tkm, and 1.22 kg, respectively when the other factors are unchanged based on the Equation 6. The breakeven points of various electricity sources indicate that oil has the lowest quantity and nuclear has the highest. This is because oil has highest unit global warming potential, and nuclear has the lowest. All outcomes for CO_2 natural wollastonite payback analysis are positive, which means the total carbon emission is less than the carbon captured. Therefore, using the natural wollastonite for carbon sequestration is a carbon negative approach.

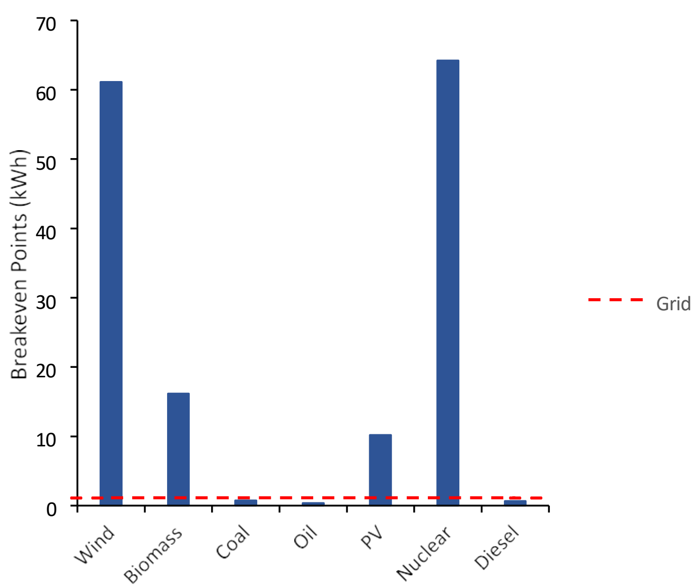

Figure 8. Breakeven points of various electricity types for natural wollastonite scenario.

For the synthesis scenario, transportation, diesel for spreading, and seven types of electricity (grid mix, wind, biomass, coal, oil, PV, and nuclear) of 60% production rate are elements to calculate balance points. Fig. 6 illustrates the results of the breakeven analysis for the synthetic wollastonite scenario based on seven types of electricity. The CO_2 payback period of transportation and diesel are -518,361.70 tkm and -142.15 hours, respectively. Additionally, the various production rate for synthesis is considered. the quantity of chemicals for wollastonite synthesis cannot change due to the constant molar mass of chemicals, hence the raw materials are neglected in breakeven calculations, but the amount of chemicals is included for other parameters' payback estimation. The payback of all outcomes are negative regarding different production rates, which means all inputs for carbon neutral are less than zero. This is because the total carbon emissions from raw materials to spreading are always larger than the carbon sequestrated. The CO_2 payback results for 80% and 99% production rate are still negative, whereas the higher production rate has higher CO_2 payback period regardless of the electricity type. Therefore, the synthesis wollastonite is not beneficial from a carbon dioxide sequestration.

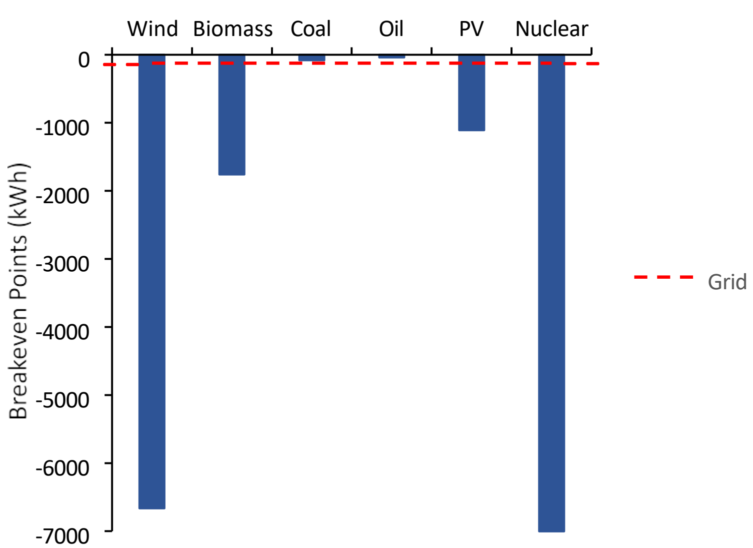

Figure 9. Breakeven points of various electricity types for synthetic wollastonite scenario (60% production rate).

2.7.3. Sensitivity analysis

A comparison of the overall impact of the seven electricity resources for natural wollastonite scenario and synthesis scenario is illustrated in Table A3, Table A4, and Fig. 7. For the natural wollastonite scenario (Fig. A1), the renewable energy resources, especially wind, biomass, and nuclear, contribute the least implications in most environmental and human health categories. However, biomass is a precursor to the SM because it can emit more than 90% of surface NO_2 during combustion, and NO_2 is the primary source to form O_3 through photolysis (Khodmanee and Amnuaylojaroen, 2021). Unsurprisingly, fossil fuel-based energy resources (e.g. coal, oil) are polluters to all environmental and human health indicators, except SM. The percentage contribution of each electricity resource associated with other life cycle stages in all ten environmental and human health impacts is demonstrated in Fig A1. Transportation shows a high impact contribution in the OD, GW, EU, HHc, HHnc, RE, ET, and FFD of the grid, wind, biomass, PV, and nuclear, whereas loading operation is a majority in SM and AC. Nevertheless, electricity for wollastonite crushing that used coal and oil as inputs dominated implications in EU and HHc, and OD and GW, respectively. In the synthesis scenario, the 60% production rate is representative to explain the relationship between life cycle stages associated with various energy resources and environmental and human health impacts (Fig. A2). The “sustainable” electricity resources are the same as the natural scenario, which is prevailed by wind, biomass, and nuclear. Besides, not only do fossil fuel based resources contribute the highest impact for most implications, but also grid dominates impacts in EU, RE, and ET.

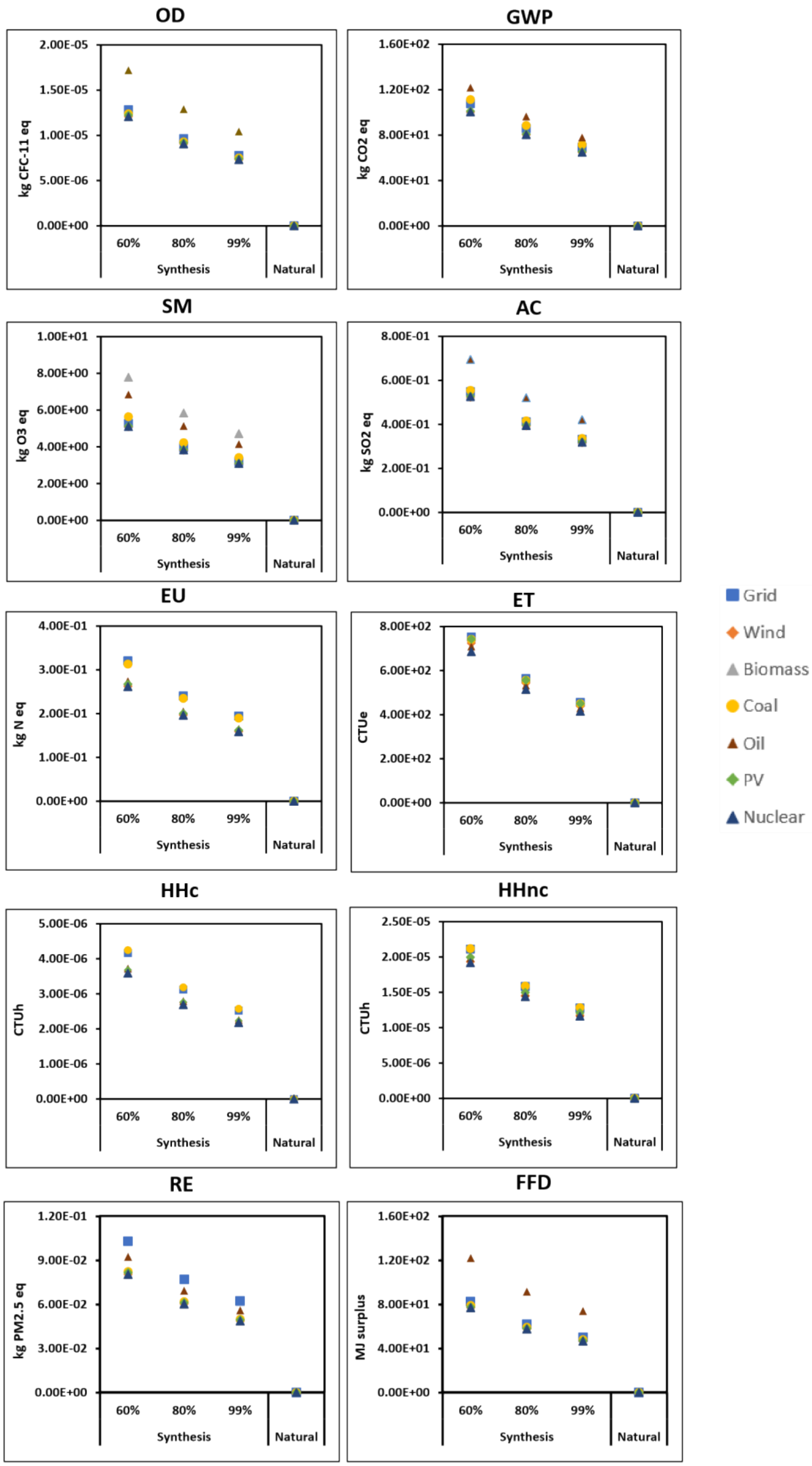

Figure 10. Impact comparison of two scenarios based on different electricity resources.

2.8. Discussion

As discussed previously, the current work contributes to the LCA literature on EW by comparing emissions of natural and synthetic wollastonite from the product's life cycle. For natural wollastonite, findings from this research were consistent with the published literature, in which the majority of environmental and human health impact categories identified transportation as a hotspot (Koornneef and Nieuwlaar, 2012; Lefebvre et al., 2019). The environmental and human health implications for synthetic materials, especially wollastonite, have not been analyzed in previous literature. Therefore, this is the first comprehensive LCA study done for the EW supply chains (raw material acquisition, manufacturing and spreading rock dust) associated with the end-of-life stage for both natural and synthetic wollastonite. Based on the results presented above, natural wollastonite has better performance in all environmental and human health impact indicators including CO_2 payback period that comparing synthetic scenario regardless of yield rate, hence the natural wollastonite should be utilized for carbon capture when considering the tradeoffs of selecting synthetic and natural wollastonite.

In this study, the CO_2 removal rate is based on stoichiometry, but the particle surface area can affect the removal efficiency as well. According to the relationship between reaction rate and particle surface area, the absorption rate is proportional to surface area, which means the absorption rate is increased when the surface area of the particles increases in the same unit time (Wang et al., 2022; Yang et al., 2010), hence the sequestration rate has the potential to be accelerated by using high surface area particles (Haque et al., 2020b; Renforth, 2012; Rigopoulos et al., 2018). The range of surface area for natural wollastonite powder is between 0.142 m^2/g to 20.28 m^2/g when mixed with soil to capture CO_2 on cropland (Haque et al., 2020a; Wood et al., 2023). The surface area range is quite large if wollastonite is mixed with cement, which is between 0.2 m^2/g to more than 1000 m^2/g (He et al., 2020; Khan and Ashraf, 2019; Ramézani et al., 2021). The surface area of synthetic and natural wollastonite that used in this study is 40.69 m^2/g (Huang and Chang, 2009) and 20.28 m^2/g (Haque et al., 2019), respectively(Haque et al., 2019; Huang and Chang, 2009). Since the surface area of synthetic wollastonite is two times larger than natural ones, the removal efficiency of synthetic wollastonite is two times higher than natural wollastonite in the same unit time. Additionally, the silicate mineral dissolution rate can be affected by temperature (Banwart et al., 2009; Bertagni and Porporato, 2022). The higher temperature accelarates the mineral dissolution rate at warmer temperature (Banwart et al., 2009), EW applications are best suited for regions that are mostly temperate-humid and tropical because the weathering of minerals, particularly silicates, requires a soil environment that is adequately warm and wet (Bertagni and Porporato, 2022).

A possible improvement to reduce environmental and human health impacts is deploy the clean transport technologies, such as the renewable transport fuels (Koornneef and Nieuwlaar, 2012). Besides, the sifted and manufactured calcium silicate from construction and demolition (C&D) waste can reduce the demand for raw materials extraction significantly (Eufrasio et al., 2022). When compared to aggregates made from raw crushed stone material, the use of recycled C&D waste can reduce greenhouse gas emissions by 65%, and it is consistent with the circular economy's goal of turning waste into resources and extending the useful life of commodities

(Eufrasio et al., 2022). To reduce the need for mining, grinding and manufacturing, innovative ERW uses C&D waste is need a separate LCA analyses to determine the likely reductions in resource depletion, as well as the environmental and health implications (Eufrasio et al., 2022). For carbon capture and utilization (CCU), the products, calcium carbonate, from EW can be the alternative raw material to process cement that applied in construction (Hargis et al., 2021). This system can be a closed-loop approach as cradle-to-cradle assessment to improve the environmental sustainability.

There are several limitations to this work. Firstly, not all relevant environmental impacts are taken into consideration in LCAs. For example, spreading of wollastonite increase the atmosphere particular that cause lung diseases (Koornneef and Nieuwlaar, 2012; Normohammadi et al., 2016). A further limitation is if the scope of this study was extended and the necessary production of chemical fertilizer were considered with EW, the final results may change because of fertilizer usage. Moreover, due to the major assumption in literature or stochasticity in real world, this study may not be representative of the actual enhanced weathering processes.

2.9. Conclusion

Critical research gaps were addressed depending on the LCA literature review of EW for carbon sequestration. In this study, comparing a synthetic and natural wollastonite scenario, it was discovered that natural wollastonite performed better in terms of environmental and human health perspectives. When shifting from natural scenario to synthesis scenario increases environmental impact and human health impacts by over 100%. However, the overall environmental and human health outcomes will reduce by 55%-68% when the production rate increases from 60% to 99%. Therefore, raw materials and methods for synthesis, technologies that are used for synthesis, and other factors that can influence production efficiency may further affect environmental and human health performances. Based upon results from the breakeven analysis, synthesis is an inappropriate approach for wollastonite acquisition, whereas natural wollastonite is suggested for carbon capture to reach neutral carbon.

Results emphasize several gaps that need additional research to solve and improve in the future. In the synthesis scenario, types of chemicals for production, chemical usage efficiency, and novel technologies can be improved and developed. The natural wollastonite scenario needs to increase accuracy that using actual data for analysis. Additionally, varied transportation may result in different environmental and human health outcomes. This study only contained the environmental sustainability perspective, hence the economic and social tradeoffs need to be estimated for enhanced weathering in the future study. For example, the net present value (NPV), benefit/cost analysis can be used to evaluate carbon capture technologies in economic perspective, and willingness-to-pay can be used to determine the human behavior and environmental attitude regarding to the carbon capture, storage and utilization technologies in social perspective.

2.10. Acknowledgement

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This work has not been formally reviewed by the sponsors and reflects the opinions of the authors.

3. Using LCA to estimate the environmental impacts of electrochemical CO reduction to acetate in bioelectrolyte for product upgrading to bioplastics

The following chapter is a revised portion of an article submitted in the Nature Synthesis and currently under review, with the citation:

Feng, D., Hicks, A.L., Using LCA to estimate the environmental impacts of electrochemical CO reduction to acetate in bioelectrolyte for product upgrading to bioplastics.

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The article appears as accepted, although style and formatting modifications have been made.

<u>Authorship contribution statement</u>

Danyi Feng: Designed Research, Performed Research, Analyzed Data, Wrote the Paper.

Andrea Hicks: Designed Research, Revised the Paper.

3.1. Abstract

Electrochemical CO_2/CO reduction typically stops at C2 to C3 products, and it is getting extremely challenging to obtain high-value hydrocarbons that are longer than C3. Integrating electrochemical CO_2/CO electrolyzers with a downstream bioreactor could help to obtain highvalue long-chain products, but the electrolytes are mismatched in these two systems preventing a smooth integration. Here we demonstrated a porous solid electrolyte (PSE) electrolyzer producing highly selective and pure acetate that coupled with the biosynthesis system to generate C4+ polyhydroxybutyrate (PHB) bioplastic. To understand the environmental viability of integrating CO_2RR with biosynthesis technologies for PHB production, the life cycle assessment (LCA) was conducted to quantify the environmental implications associated with cradle-to gate life cycle stages. The results reported that the electrochemical process is the main contributor to

all impact indicators.

3.2. Introduction

Upgrading CO_2 captured from point sources or directly from air is one of the promising technologies to mitigate climate change (Aresta et al., 2014; Xia et al., 2019). Among different CO_2 utilization technologies, the electrochemical CO_2 reduction reaction (CO_2RR), with the energy input from renewable electricity, has shown great promise in producing a wide range of valuable products, particularly high-value C2+ liquid products such as acetate, ethanol, and npropanol (Ji et al., 2022; P. Wang et al., 2022; X. Wang et al., 2022). However, it becomes more difficult when targeting carbon chains longer than four carbons (C4+). On the other hand, biosynthesis systems were demonstrated to upgrade CO_2 or its derivatives (such as carbon monoxide) into energy-intensive and long-chain carbon fuels and chemicals, such as n-butanol and polyesters (Li et al., 2012; Pohlmann et al., 2006). However, the bio-upgrading system could suffer from low overall energy efficiency and carbon utilization efficiency when directly fed with CO_2 or low-grade CO_2RR products, making the whole CO_2 utilization process not economically nor practically feasible (Haas et al., 2018).

An optimized integration of electrochemical CO_2RR with biosynthesis could avoid this challenge and upgrade CO_2 to longer carbon chain and higher value products in an energy-efficient way (Crandall et al., 2023; Zheng et al., 2022). Instead of CO or formate as low-grade CO_2RR products from electrocatalysis (Dongare et al., 2021; Fan et al., 2020; Jiang et al., 2018), acetate, a widely observed CO_2/CORR product on Cu-based catalyst, is a preferred carbon source to bioreactors as it can be more effectively digested by bacteria to produce high value products (Zheng et al., 2022). C1 products, such as formate, can also be used as carbon sources for microbial reactions to product upgrading. However, carbon sources normally need to convert into acetate first to be used as a precursor (acetyl-CoA) for longer carbon chain products or energy sources like ATP in the bioreactor (Roh et al., 2021; Rowaihi et al., 2018; Stöckl et al., 2020). Acetate molecules can easily form acetyl coenzyme A (acetyl-CoA) by acetyl-CoA synthetase presented in bacteria species, which is an ideal precursor for various complex molecules in the biosynthetic process (Liu et al., 2015). Direct feeding the acetate can decrease the reaction steps inside the bioreactor, enhancing reaction activity and efficiency (Claassens et al., 2019). Here we demonstrated a porous solid electrolyte (PSE) electrolyzer producing highly selective and pure acetate that coupled with the biosynthesis system to generate C4+ polyhydroxybutyrate (PHB) bioplastic.

To effectively evaluate the environmental viability of integrating CO_2RR with biosynthesis technologies for PHB production, it is essential to conduct a comprehensive life cycle assessment (LCA). The LCA study would provide a holistic view of the potential impacts associated with the entire lifecycle, from raw material extraction through production to disposal (Feng and Hicks, 2023). Kachrimanidou et al. (2021) assessed the environmental implications of 1 kg of PHB production using sunflower meal as a carbon source. The findings presented the biorefining of sunflower meal and crude glycerol results in sustainable PHB production for carbon emissions. Rueda et al. (2023) analyzed the potential impacts of 1 kg PHB production using inorganic carbon as a carbon source from cyanobacteria based on various PHB contents (15%, 35%, and 50%). The results showed that increasing PHB content reduced the environmental impacts, especially the content between 67% and 75%. The main contributor to all environmental indicators is cultivation-construction materials for PHB extraction from bacteria. Kookos et al. (2019) compared the environmental implications of using various carbon sources for producing 1 kg PHB with those of HDPE. The results reported that using sugarcane as a carbon source has the lowest carbon emissions and corn sugar has the highest for PHB production, even though the carbon emissions using corn sugar are higher than HDPE. Koch et al. (2023) compared the environmental impacts of using corn feedstock and CO_2 feedstock as carbon sources for polyhydroxyalkanoate (PHA) production. The findings indicated that using the photoautotrophic production route for PHA production from CO_2 is a promising technology with favorable environmental impacts, especially when compared with heterotrophic production that relies on glucose as a feedstock. However, none of these studies have considered using CO_2/CO as feedstock to produce PHB.

The purpose of this study is to quantify the environmental and human health impacts of PHB production using carbon monoxide (CO) as feedstock via electrochemical and biosynthesis processes.

3.3. Method

3.3.1. Goal and scope

The aim of this LCA study is to estimate the environmental and human health implications of bioplastic using CO as feedstock. The functional unit (FU) is 1g of bioplastic produced. The bioplastic is assumed to be a single use product, with a somewhat unknown end of life disposition. Therefore, a cradle-to-gate assessment is performed, which implies that the system boundary encompasses all life cycle stages leading up to and including the production phase of the raw bioplastic. The system boundary includes electrochemical and biosynthesis processes, as presented in Figure 8.

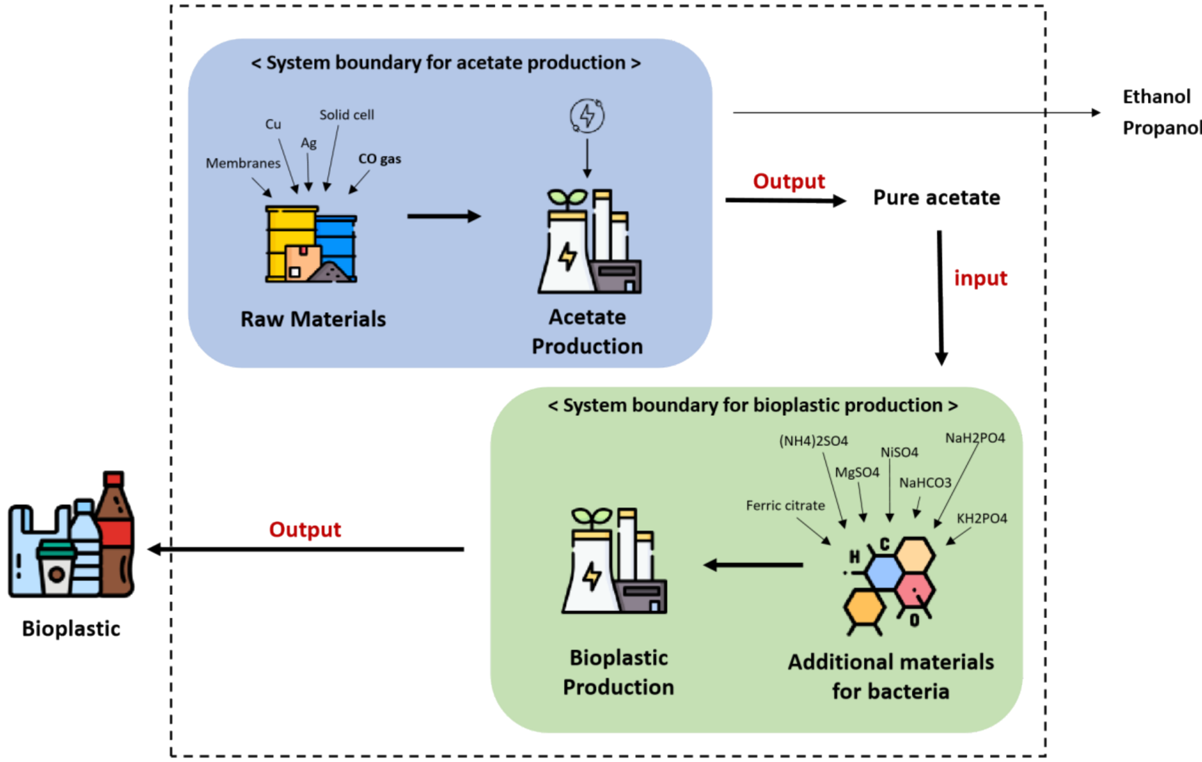

Figure 11. System boundary to produce bioplastic based on electrochemical and bio-synthesis processes.

3.3.2. Life cycle inventory

Electrochemical process. A detailed inventory of the electrochemical process can be found in Table B1. The production of extremely pure acetate is achieved by employing electrocatalytic CO reduction (CORR). Numerous electrocatalysts are capable of converting CO_2 gas into CO gas with high efficiency (near 90%). Therefore, utilizing CO gas for the production of valuable products presents novel prospects. The flow rate of CO gas is 4-5 sccm, and the average gas flow rate (4.5 sccm) is used. The DI water flow rate is 1 mL/min, while the total duration of this experiment is 40 hours. The solid cell system is developed to produce pure acetate liquid directly. In the cell, the cathode and anode consist of gas diffusion layer (GDL) electrodes coated with catalysts, with anion and cation exchange membranes (AEM and CEM) as the separators between them. The 2.25 cm^2 Sigracet 28 BC carbon fiber paper is a GDL electrode that acts as the substrate for catalyst deposition. Polymerized acrylonitrile is the raw material of carbon fiber paper and the unit weight is 105 g/m^2 (Fuel Cell Store, n.d.), so the total weight of carbon fiber paper used in this solid cell system is approximately 0.024 grams. A Nafion membrane and AEM are used for cation and anion exchange, respectively. A Cu-Ag mixed catalyst is coated on the electrode. The actual weight of Cu and Ag is 0.974 mg and 0.826 mg, respectively. Additionally, a 3g Amberchrom 50WX8 is utilized as a solid electrolyte, and the matrix is polystyrene crosslinked with divinylbenzene (Supelco, 2023), hence the polystyrene is used as the inventory from the inventory databases. 400 mA/cm^2 electricity is applied to obtain 2686 ppm acetate. Besides, 308.7104 ppm ethanol and 65.2838 ppm propanol are by-products from the experiment.

Bio-synthesis process. Inventories of the bio-synthesis process are shown in Table B2. *Ralstonia eutropha* is used to divert carbon flow to biomass and multi-carbon products (e.g., PHB) because it can grow on acetate that is produced from an electrochemical reaction. The total volume for incubating *Ralstonia eutropha* is 40 mL, including 6.74 g/L $Na_2HPO_4 \cdot 7H_2O$, 1.5 g/L KH_2PO_4, 0.167 g/L $(NH_4)_2SO_4$, 80 mg/L $MgSO_4 \cdot 7H_2O$, 1 mg/L $CaSO_4 \cdot 2H_2O$, 0.56 mg/L $NiSO_4 \cdot 7H_2O$, 0.4 mg/L ferric citrate, and 200 mg/L $NaHCO_3$. The average acetate consumption is 33.5 mM, and the average hydroxybutyrate production rate is 4.4 mM under 4 days experiment. However, potassium dihydrogen phosphate (KH_2PO_4) and ferric citrate have not existed in any inventory databases (e.g., ecoinvent), so the utilized reactants involved in the synthesis of these four chemicals are employed to assess the implications of these four products based on stoichiometry.

KH_2PO_4 is formed by a reaction between potassium carbonate and phosphoric acid (Han et al., 2020):

$$K_2CO_3 + 2H_3PO_4 \rightarrow 2KH_2PO_4 + H_2O + CO_2\uparrow \qquad \text{Equation 7}$$

The Gurr~ and Ridge (1991) reported that the ferric citrate is prepared and produced by ferric chloride and citric acid:

$$FeCl_3 + C_6H_8O_7 \rightarrow C_6H_5FeO_7 + 3HCl \qquad \text{Equation 8}$$

3.3.3. Life cycle environmental and human health assessment

Ecoinvent and USLCI inventories, along with the TRACI (version 2.1) method, are utilized in conjunction with SimaPro software (version 9.2.0) to analyze the environmental and human health impacts. The analysis covers ten midpoint categories, including seven environmental impacts: ozone depletion (OD, kg CFC-11 eq), global warming potential (GWP, kg CO_2 eq), smog (SM, kg O_3 eq), acidification (AC, kg SO_2 eq), eutrophication (EU, kg N eq), ecotoxicity (ET, CTUe), and fossil fuel depletion (FFD, MJ surplus). Additionally, three human health indicators are considered: carcinogenic effects (HHc, CTUh), non-carcinogenic effects (HHnc, CTUh), and respiratory effects (RE, kg PM2.5 eq) (Feng and Hicks, 2023). The TRACI method, developed by the U.S. EPA, adopts a midpoint approach that relies on reliable and transparent data and models sourced from within the United States (Ghamkhar et al., 2022c).

3.4. Results

Table B3 presents the characterization results of two manufacturing processes for 1g bioplastic (PHB) production including the carbon source gas production used in the laboratory scale synthesis (modeled as CO_2). The impact of producing 1 g of the plastic, the overall environmental impact is 1.65e-3 kg of CO2e. Of this the vast majority of impact occurs during the electrochemistry portion of the life cycle, with the biosynthesis process contributing a minimal amount. These results stop at the synthesis and do not include the further refining and separation of the plastic material from the microbes utilized in the biosynthesis portion. When moving the production stage from the electrochemical process to the bio-synthesis process, the environmental and human health implications decreased by more than 100%. Overall, the electrochemical process has worse performance than the biosynthesis process from both environmental and human health impacts. The characterization results of bioplastic production associated with electrochemical and bio-synthesis processes for 1 FU produced without CO gas manufacturing are shown in Table B4. CO gas is excluded specifically because CO_2 is assumed as the raw material to produce bioplastic and sourced from waste products and thus is free environmentally. When comparing the implications associated with CO production, utilizing CO as a waste product to produce bioplastic demonstrates better performance in terms of both environmental and human health impacts. It results in a percentage decrease of 99% considering the CO_2e perspective.

Generating bioplastic from CO is an important technological step with respect to making bioplastics out of waste CO_2 while also reducing dependence on petrochemical sources for plastic. It also provides an opportunity to create a valuable product from captured CO_2. At the same time, it is critical to understand the environmental and human health impacts and implications of these processes at early technology maturity levels. Selected environmental and human health impacts are presented in Figure 9, including global warming potential, eutrophication potential, and non-carcinogenic human health impacts, the remainder of the impact categories considered are presented in the Appendix B (Figure B1). At present for each gram (FU) of bioplastic produced, 1.5E-05 kg of CO_2 is produced due to the consumption of chemicals, electricity, etc., when the generation of CO is not included. However, based on the stoichiometry of the reactions, 10.8 kg CO is incorporated into the bioplastic produced for 40 hours experiment and 16.97 kg of CO_2 can be transformed into CO gas. This means that at the current technology level, this process utilizes the captured CO_2 effectively as it involves a higher consumption of CO_2 compared to the amount emitted. Therefore, this technology not only mitigates the additional impact of petroleum plastics but also contributes to achieving carbon neutrality. It should be noted that in this analysis the CO is considered to be a waste produced provisioned by another process, and thus is considered “free” environmentally.

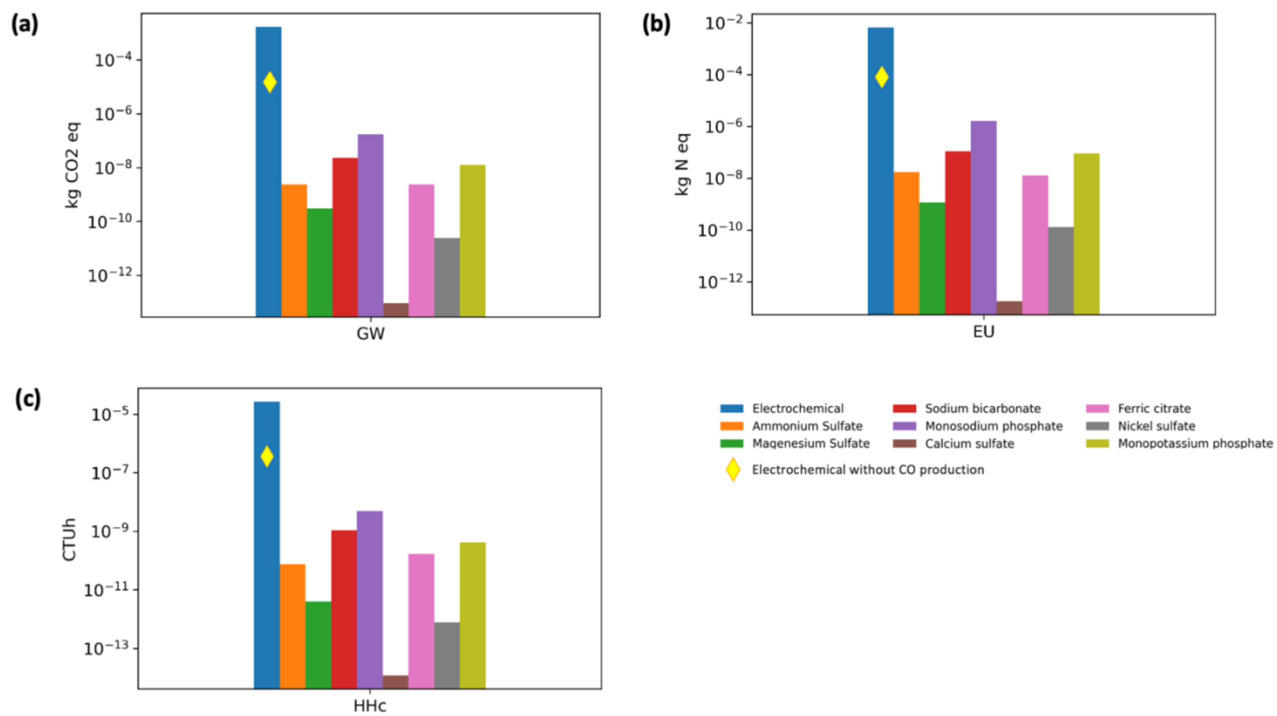

Figure 12. The life cycle distribution of two processes for (a) global warming potential, (b) eutrophication, and (c) human health carcinogenic based on the log scale. The y-axes are plotted on a logarithmic scale for 1 FU.

3.5. Discussion

The study estimates the environmental and human health impacts of two manufacturing steps in a process for producing 1 gram of bioplastic (PHB): electrochemical and subsequent biosynthesis steps, using CO as a carbon source. The electrochemical process has worse environmental and human health performance. When excluding CO gas production and assuming CO_2 as a wastederived raw material, the production of bioplastic from waste CO_2 shows a dramatic reduction of over 99% in environmental and human health impacts. The study emphasizes the importance of evaluating these impacts at the early stages of technological development to ensure sustainable progress. In essence, the question is whether to include the production of CO gas in the analysis, which is what occurs at the laboratory scale. Or to consider the more likely actual production of this plastic, using CO_2 as a free waste source.

Although the process is anticipated to use captured CO_2 effectively, incorporating 10.8 kg of CO into the bioplastic for every 40-hour experiment and transforming 16.97 kg of CO_2 into CO gas, there are still net CO_2 emissions. For each gram of bioplastic produced, 1.5E-05 kg of CO_2 are emitted due to the consumption of chemicals and electricity. Therefore, while the process makes substantial progress towards carbon neutrality, it does not achieve a completely carbon-negative status at this stage. Further optimization and advancements are necessary to reduce these emissions and move closer to a true carbon-negative outcome, such as utilizing renewable electricity resources.

When comparing the bioplastic production process to conventional plastic production, significant differences in environmental impact become evident. Traditional plastics, such as polyethylene (PE) and polypropylene (PP), are derived from petrochemicals and have a substantial carbon footprint. According to Spierling et al, (2018), the production of 1 kg of conventional plastic typically results in the emission of approximately 2 to 3 kg of CO_2. In contrast, the bioplastic production process outlined in this study, while incorporating captured CO_2, results in higher CO_2 emissions with 1.5E-05 kg of CO_2 emitted for every 1 kg of bioplastic produced due to the large consumption of chemicals and electricity. However, it is important to note that this study was conducted on a laboratory scale. If scaled up to commercial levels, process optimizations and economies of scale could significantly reduce CO_2 emissions, potentially making bioplastic production more competitive with traditional plastics. Further improvements in production efficiency and the integration of renewable energy sources are necessary to enhance sustainability and reduce the carbon footprint of bioplastic production, making it a truly viable alternative.

3.6. Conclusion

In this study, the environmental and human health implications of the electrochemical and biosynthesis processes for bioplastic production are estimated utilizing LCA methodology. It was discovered that the electrochemical process contributes the most to environmental and human health impacts. It is important to note that the processes are not currently carbon-negative. Therefore, the environmental and human health performances can be further influenced by factors such as the raw materials and technologies used in acetate production, the experimental duration, and the efficiency of acetate obtained. Despite using CO_2 as a raw material, the bioplastic production process is currently not carbon-negative. The energy-intensive nature of both the electrochemical and biosynthesis processes, often reliant on fossil fuels, results in significant CO_2 emissions. Consequently, the overall carbon footprint of bioplastic production remains positive.

This work contains several gaps that need to be solved and improved in future research. Firstly, because of substantial assumptions made based on stoichiometry for chemicals that are used for bacteria growth, this study might not accurately represent the actual implications of the chemicals. Moreover, one potential improvement is to replace CO gas with CO_2 gas for acetate production to reduce environmental and human health impacts. This study only considered the environmental impact perspective; hence the economic trade-off needs to be analyzed for bioplastic production regarding carbon utilization in future study.

3.7. Acknowledgement

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4. Consumer willingness to pay for bioplastic produced from captured carbon dioxide

The following chapter has been submitted for consideration for publication with the citation:

Feng, D., Hicks, A.L., Consumer willingness to pay for bioplastic produced from captured carbon dioxide. In revision.

The article appears as submitted, although style and formatting modifications have been made.

Authorship contribution statement

Danyi Feng: Designed Research, Performed Research, Analyzed Data, Wrote the Paper.

Andrea Hicks: Designed Research, Revised the Paper.

4.1. Abstract

Fossil fuel-based plastic contributes to large scale environmental pollution (e.g., CO_2) and contaminants (e.g., microplastics) during the manufacturing and disposal stages. Emerging technologies that use captured carbon sources as raw materials to produce bioplastic have the potential to reduce these impacts. However, understanding consumer willingness to purchase these novel products and determining the most effective marketing strategies are required prior to widescale adoption. This study investigated the factors that influence the preference of consumers to buy captured CO_2-based single-use bioplastic water bottles. The attitude and willingness to pay are the key outcomes. The findings from two surveys indicated the participants have positive attitudes toward bioplastic water bottles, and more than half of them are willing to pay more for bioplastic water bottles compared to conventional ones. Results such as these are necessary for industry and policymakers to understand the potential of how to increase the adoption of these products.

4.2. Introduction

Plastic is a ubiquitous material commonly sourced from fossil fuels and utilized for a myriad of modern day applications. Approximately 9,200 million metric tons (Mt) of plastic have been produced in the past 50 years, with 360 million Mt of plastic generated globally in 2020 (Fischbach et al., 2022; Pathak et al., 2023; Walker and Fequet, 2023). Around 500 Mt CO_2 eq greenhouse gases (GHG) are emitted for plastic production, which is 1% of the global total of GHG emissions (Jin et al., 2023). However, if plastic production continues using current technologies and carbon sources from petroleum, the GHG emissions contribution will reach 15% of the whole industrial sector by 2050 (Jin et al., 2023). Therefore, it is urgent to develop alternative plastic materials. Consequently, carbon capture and utilization (CCU) technologies are one potentially sustainable method to reduce the global CO_2 emissions of plastic production by sourcing plastic from CO_2, thereby transforming plastic production into a carbon sink. For renewable plastic production, several thermochemical (Kuusela et al., 2021) and direct conversion pathways are currently being developed (Grignard et al., 2019; Salehizadeh et al., 2020a), utilizing CO_2 as the carbon feedstock and hydrogen as both the co-reactant and primary energy vector with heat, electrons, or irradiation (Alper and Yuksel Orhan, 2017). Grignard et al. (2019) provided a comprehensive review of CO_2-derived polymers for sustainable and novel plastic materials development, detailing innovative methods and strategies for transforming CO_2 directly or through intermediates into a diverse array of macromolecules with specific properties. This represents a notable advancement in reducing carbon emissions within plastic manufacturing processes. Additionally, CO_2 fixation is one of the CCU methodologies, which converts CO_2 removed from the atmosphere to chemicals such as organic acids (Carpine et al., 2020; Fabien et al., 2021; Salehizadeh et al., 2020b). Acetic acid can be defined as a CO_2-derived organic acid and as an alternative carbon feedstock for use in polyhydroxy butyrate (PHB) production via electrochemical or thermos-catalytical reduction processes, thereby closing the bioplastic carbon cycle (Garcia-Gonzalez and De Wever, 2018; Vlaeminck et al., 2022; Wang et al., 2019). Besides, the price per kg of CO_2 is cheaper than other carbon sources per unit for bioplastic production (Jo et al., 2021), especially when CO_2 is derived from industrial flue gas (Sirohi et al., 2021).

Bioplastic made from captured CO_2 is an innovative solution that contributes to environmental sustainability by utilizing GHGs as raw materials. Polyhydroxybutyrate (PHB) is one of the biodegradable polymers in the PHA family that are most commonly applied in packaging industries, agriculture, and medical fields. PHBs are produced by various microorganisms (e.g.

Cupriavidus nectar, Methylobacterium rhodesianum, Bacillus megaterium) under conditions of limited nutrition, utilizing carbon sources for energy (Atiwesh et al., 2021; Getachew and Woldesenbet, 2016; McAdam et al., 2020; Rostkowski et al., 2012). While these plastics are typically derived from biomass carbon sources (e.g., sunflower, soybean oil) (Kachrimanidou et al., 2021; Kookos et al., 2019), there is also potential for production using alternative carbon sources, such as captured CO_2. Therefore, bioplastic made from captured CO_2 is considered a potential sustainable solution as it utilizes GHGs as a carbon source resource, thus reducing the overall carbon footprint and contributing to the mitigation of climate change by transforming CO_2 from an environmental liability into a valuable material (Atiwesh et al., 2021; Zwicker et al., 2023).

Despite the numerous advantages, the global bioplastics market has experienced limited growth and competition. This is primarily due to the higher production costs per unit compared to conventional petroleum-based plastics, resulting in reduced competitiveness for manufacturers compared to traditional plastic producers who benefit from established supply chains and economies of scale (Hwang et al., 2021; Notaro et al., 2022a), limited availability and insufficient product information are among the significant barriers hindering the growing demand for bioplastic products. Besides, high prices and ineffective marketing activities have been identified as factors impacting the sales volumes of bioplastic products (Lettner et al., 2017). Determining the factors that drive consumer adoption and purchases is crucial for the development of the bioplastic product market. However, only a limited number of studies have investigated these factors. Scherer et al. (2018) determined the consumer preferences for a biobased plastic water bottle for bicycles and a running shoe with a bio-based sole in Germany, which utilizes crops as raw material including soybean oil from the USA, palm oil from

Indonesia, rapeseed oil from Germany, and castor oil from China. Additionally, this study provided three price levels for each product: €6, €8 and €10 for the water bottles, and €89, €99 and €109 for running shoes. The results demonstrated that respondents preferred to purchase biobased plastic products due to the substantial CO_2 emission reduction. While there was a general interest in bio-based sample products, the respondents preferred the lowest-priced options for purchasing bio-based products, finding them to be the most cost-effective, while they considered the medium price range acceptable due to a reasonable cost-performance ratio. Respondents showed a strong preference for products that significantly reduce CO_2 emissions, particularly those that offer a 60% reduction in CO_2 emissions during manufacturing. De Marchi et al. (2020) surveyed consumer preferences and willingness to pay (WTP) for plastic water bottles in Italy, including those made of conventional plastic polymers and environmentally sustainable alternatives (e.g., bio-polyethylene terephthalate (PET), polylactic acid (PLA)), focusing on how consumer choices might be influenced by sustainability information when comparing two experimental scenarios. The results indicated that Italian consumers were willing to pay more for bio-based water bottles made from PLA compared to common PET bottles. Moreover, consumers preferred virgin plastics that are whether they are petroleum or bio-based over recycled materials and the provision of information does assist consumers in distinguishing between different types of plastics but does not substantially increase their WTP. Skouloudis et al. (2023) highlighted that more than 40% of Greek respondents indicated their WTP more for polyhydroxyalkanoate (PHA) bioplastic bottle, a pack of breadsticks containing phenolic extracts derived from olive mill wastewater as an ingredient, and bio-nylon jackets compared to the conventional plastic bottles, breadsticks, and nylon jackets. Zwicker et al. (2023) reported that survey participants showed positive attitudes toward bio-based plastics (polyethylene furanoate (PEF) and paper PEF), indicating a WTP premium for them. Regardless of being under observation, they overwhelmingly expressed a preference for bio-based bottles. Consumer decisions to buy bioplastic products have been determined to be influenced by consumers' intentions, eco-friendly consumer values, attitudes toward bioplastics, altruism, subjective norms, innovativeness, and socio-demographic characteristics including age, gender, education, and income (Notaro et al., 2022a).

In the United States, the total sales for beverage packaging units reached $195 billion in 2013 (Kang et al., 2017), and the annual consumption of single plastic water bottles per capita notably amounts to 50 billion units (Bruchmann et al., 2021). This substantial annual water bottle demand associated with the environmental impacts of CO_2 emissions in the production and disposal of these bottles led to the selection of single-use bioplastic bottles made from captured CO_2 for this study, emphasizing the opportunity for a significant market transition to more sustainable options (Zwicker et al., 2023b). Therefore, it is important to identify the factors that could affect consumers' decisions to shift towards more environmentally friendly materials, particularly considering that the majority of consumers frequently encounter and purchase bottled waters and other beverages.

4.3. Methods

4.3.1. Survey instrument and implementation

WTP data used in this study are collected from two social surveys to estimate the willingness to purchase plastic bottles made from CO_2-captured bioplastic and the awareness of climate change in the United States. Both surveys were approved by an Institution Review Board (IRB) of the

University of Wisconsin-Madison. The first more robust survey (Survey 1) was distributed to the public through various pathways (e.g., mailing list, online posting) using the Qualtrics online survey platform from March 20th to June 25th, 2023. The second less robust and shorter survey (Survey 2) was distributed in the Science Expedition at the University of Wisconsin-Madison on April 6th, 2024.

Survey 1 includes four sections and a total of twenty-five questions consisting of 1) climate change awareness, 2) perceived knowledge about carbon capture and utilization (CCU) products, 3) CCU product purchase behavior, and 4) socio-demographic information. Section 1 determined consumer beliefs and concerns about CO_2 emissions. Section 2 focused on the knowledge background of CCU products, such as listing the products made by captured carbon. Section 3 asked the consumer preferences and WTP for single-use bioplastic bottles. Section 4 collected socioeconomic and demographic information, including the respondents' age, gender, race/ethnicity, education level, occupation, household annual income, and environmental consciousness. Survey 2 only includes four questions, including the highest price of single-use bioplastic water bottles respondents are WTP, consumer beliefs about climate change, and consumers' attitudes towards the environment. These two survey instruments and information regarding their administration can be found in the Supporting Information (Appendix C).

4.3.2. Analysis

The XGBoost and logistic regression (LR) are selected to classify the data according to WTP and purchase behaviors. XGBoost, a powerful machine learning algorithm for gradient boosting, is employed to extract and select informative features from the training dataset, significantly enhancing the data's predictive ability which is then utilized as the input for training the LR (Logistic Regression) classifier.

Python is selected to run the XGBoost and LR models. Feature selection improves the efficiency of model building, enhances the capacity of the model for generalization, and reduces overfitting concerns. An effective metric for assessing feature importance should satisfy the criteria of both consistency and accuracy. Therefore, the SHapley Additive exPlanations (SHAP) value is used to evaluate the importance of features that represent its contribution to the model's output. SHAP values illustrate the impact of each feature on individual predictions, the relative importance of each feature compared to others, and the model's reliance on the interaction between features. Ten features were considered in this study, including heard of bioplastic, frequency of bringing own bottle, CO_2 products, decision to buy single-use bioplastic bottles, age, gender, education, job, income, and environmental consciousness.

4.4. Results

4.4.1. Demographic results

A total of 113 completed responses were collected in Survey 1. Detailed demographic data of this survey and comparisons with the 2020 U.S. census, including gender, age, household income, educational development, and race/ethnicity distributions, are presented in Table C1 in the Supplementary Information (SI). The provided demographics show variances from the U.S. 2020 census figures, with notable differences in the representation of age groups and educational levels, likely reflecting the student composition of the respondent pool. The SI also provides a comparative analysis with national statistics. In Survey 2, 42 respondents filled out a short survey at a live outreach event.

Recognizing the value of environmental consciousness in the discussion on WTP for bioplastic bottles is essential, as it directly influences consumer behavior and preference, and the potential for innovative materials to revolutionize the packaging industries. This perspective clarifies the role that environmental awareness plays in promoting the demand for sustainable packaging, thereby becoming a crucial element in adopting bioplastic bottles. As consumers become more knowledgeable about the environmental benefits of bioplastics compared to traditional plastics, their willingness to spend on these sustainable options increases. Figure 10 presents the environmental consciousness of respondents from Survey 1. More than half of them (52.21%) care about the environment to an extent where environmental considerations are a significant portion of decision-making, but not the sole consideration. Additionally, 28.32% of respondents hold a neutral stance on environmental concerns.

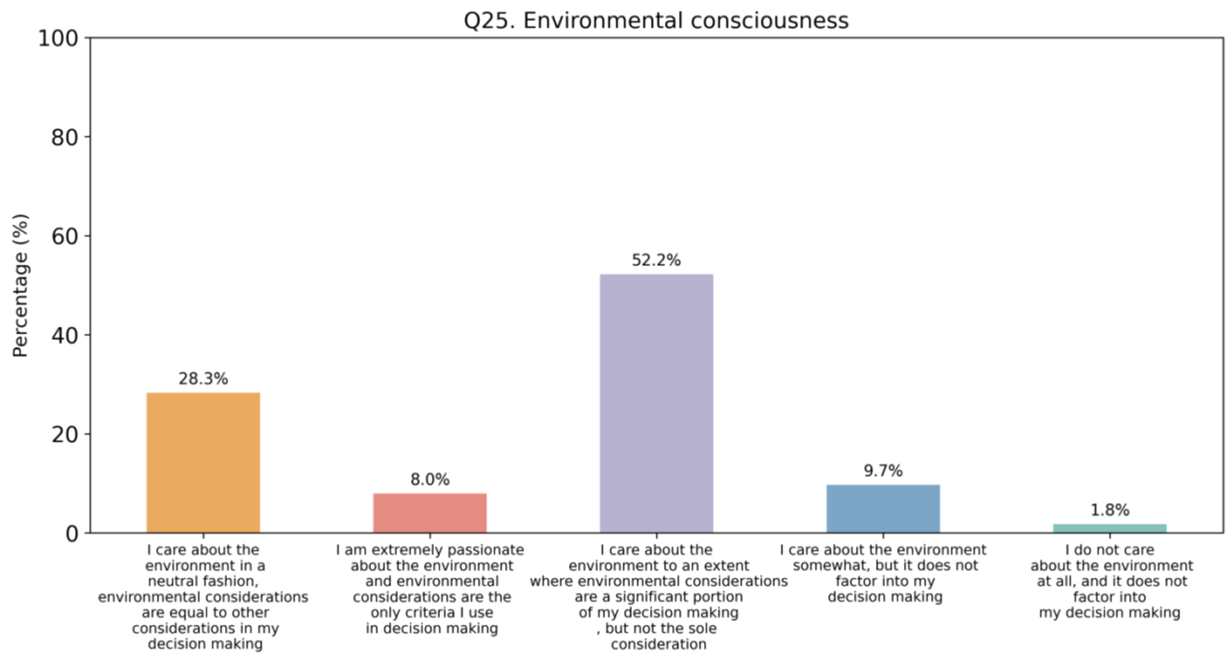

Figure 13. Percentage of environmental consciousness from Survey 1.

Figure 11 presents a diverse range of attitudes toward environmental issues, from indifference to proactive engagement, with a significant number of respondents recognizing environmental problems and willing to make personal changes to mitigate their impact. A small fraction of the respondents (4.88%) express uncertainty about the environmental information from the media, with another 13.01% believing that companies and industries have more responsibility for improving the environment than individuals do. However, a significant portion of the participants recognize the urgency of environmental issues, with 23.58% acknowledging them as critical problems to be addressed. Proactive behaviors are also evident, with 17.07% of respondents switching to environmentally friendly products and 21.95% choosing less harmful products when possible. Enthusiasm for direct involvement in environmental improvement is strong as well, with 19.51% of respondents passionate about contributing to positive change.

This result in attitudes suggests that while a segment of the population is highly motivated to make personal changes for environmental improvement, there is also a considerable portion that either undervalues these issues or feels powerless to effect change individually.

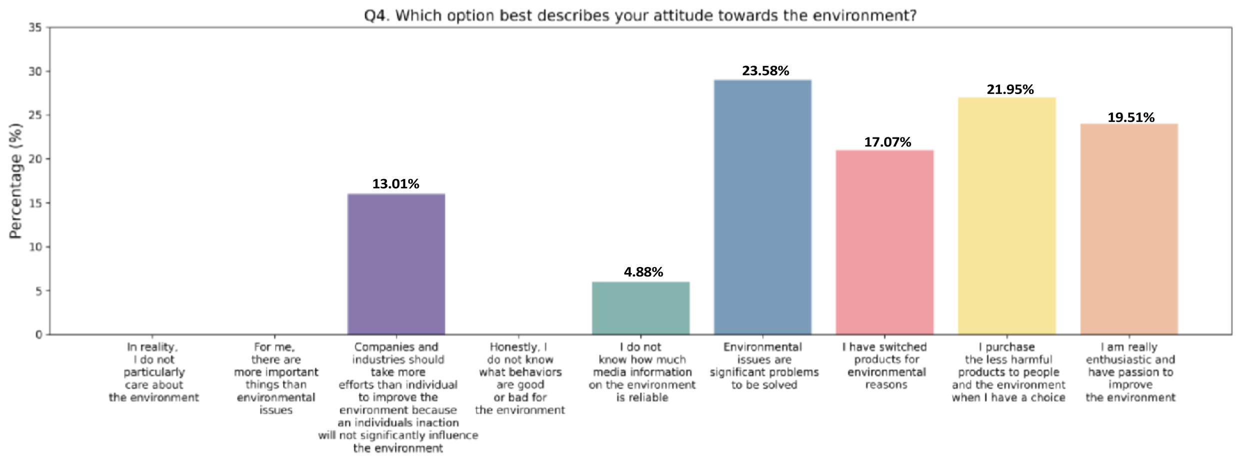

Figure 14. The environmental consciousness from the supported survey.

4.4.2. Climate change awareness

In the context of increasing climate change concerns, understanding its importance is crucial because this knowledge comprehension directly influences consumer behavior, including their valuation and WTP for products that contribute to capture carbon. The perception of climate change's urgency influences both individual and collective actions towards the environment and shapes the economic landscape by setting the value for innovations aimed at reducing its impact, like CO_2 capture technologies. This part is to determine the public awareness of CO_2 emission problem shown in Table 3. More than 80% of participants have heard about global warming and CO_2 emissions increasing and believe it is a problem currently. In addition, more than 60% of respondents were trying to reduce the CO_2 emissions in their daily lives, but approximately 21% of respondents did not have any actions to reduce their personal CO_2 emissions. The remaining 12.39% of participants are unsure whether they were actively reducing CO_2 emissions in their daily lives or not.

If respondents chose "*yes*" in question 2, the next question "*Which reason seems most significant and relevant to you*" should be answered. It was to determine the specific aspect that the respondent deems the most significant reason for CO_2 emissions, including the effects on human health, environmental impact, or the challenges it poses to socio-economic aspects of life. According to the results, the environmental impact (87.38%) is marked as the most significant and relevant reason to respondents, with 7.77% of respondents selecting human health effects. However, the participants had the least concern about the impact of climate change on the economy. Given that a previous question provided the choice to respond with '*no*', the next question "*indicate the reason that the carbon dioxide emissions issue seems irrelevant to you*" should be answered. Based on the answers provided, insufficient information (38.89%) and I can't change anything (38.89%) are the two main reasons for not realizing the CO_2 emission problem. If there were increased discussions about the notable changes in the climate over recent years, it would facilitate a better understanding of the extent of the emissions issue and the consequences of not taking action (Terjanika et al., 2022). This response "*I can't change anything*" resembles a psychological opinion of "I can't change anything, so I will not take any action." This instills particular concerns that individuals may not take any actions to reduce the emissions they generate in the near future (Terjanika et al., 2021) reported that 46% of people in 50 countries do not think climate change is a global emergency.

Table 3. Results for climate change awareness of participants from Survey 1.

	Yes	**No**	**Unsure/I don't know**
Q1. Have you heard about concerns related to increased carbon dioxide emissions and global warming?	89.23%	7.69%	3.08%
Q2. Do you believe that increased carbon dioxide emissions are a problem?	80.00%	14.62%	5.38%
Q4. Are you currently trying to reduce your personal carbon dioxide emissions?	65.63%	21.88%	12.50%

The results of two survey questions regarding climate change beliefs among participants from the supported survey are presented in Table 4. For the first question, "Do you believe climate change is real and occurring?", a significant majority, 94.62%, affirmed that they do believe climate change is real and currently happening, with none of the respondents disagreeing (0%), and only 2.38% indicating they were unsure. The second question, "Do you believe that climate change is due to the actions of people?", also received a high level of agreement, with 92.86% of participants attributing climate change to human actions. Then, no respondents outright denied this connection (0%), though a slightly higher percentage, 7.14%, expressed uncertainty. These results strongly illustrate that the vast majority of participants acknowledge both the reality of climate change and the human contribution to it, with very few respondents uncertain and none in outright denial.

Table 4. Climate change awareness results from the short survey.

	Yes	No	Unsure
Q2. Do you believe climate change is real and occurring?	94.62%	0%	2.38%
Q3. Do you believe that climate change is due to the actions of people?	92.86%	0%	7.14%

4.5. Perceived knowledge about carbon capture and utilization (CCU) products

The vast majority of respondents have a basic knowledge background of CCU products but were not familiar with them (Fig. 12). A total of 17 respondents (21.77% of the sample) have never heard of CCU products. A total of 33.87% of participants have heard about the CCU products but cannot provide a clear explanation, while 31.45% of respondents have heard of the CCU products and can give a brief definition. Only 14 participants heard of CCU products and were familiar with this and could explain what CCU product is, while only 2 respondents were very familiar with CCU products and self-reported that they can explain everything in context. Parts of the respondents have heard about captured carbon used in various fields, including building materials manufacturing (e.g., concrete), soda/vodka making, electricity/power generation, solar radiation management, oil exploitation, chemical production raw materials (e.g, producing methanol (CH_3OH)), plastic production, as well as in agriculture processing. Basic knowledge about carbon capture and utilization products plays a crucial role in shaping consumer actions, as informed individuals are more likely to support and invest in these technologies, recognizing their potential to mitigate climate change impacts. This awareness directly influences the demand for sustainable products, highlighting the importance of education in driving environmentally responsible behaviors.

A majority of respondents (62.90%) felt interested in consuming captured CO_2 as raw material to make products for use by people. A total of 14.52% and 5.65% of participants indicated that they felt delighted and prideful to use captured CO_2-based products, respectively. However, they still have respondents holding negative attitudes. Approximately 8% of participants felt worried, while 3.23% and 1.61% of respondents think CCU products are risky and disgusted, respectively.

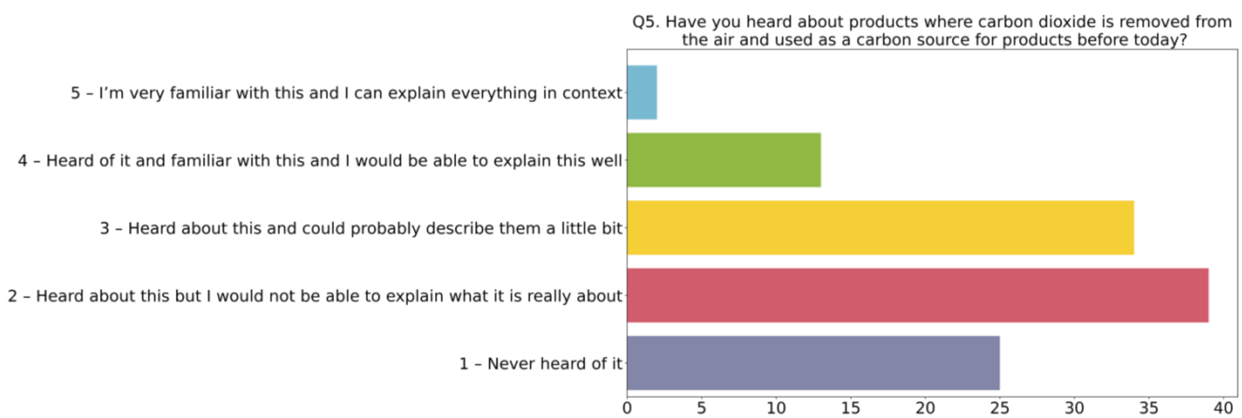

Figure 15. The results reflect the level of background knowledge participants have from hearing about CCU products.

4.4.3. CCU products purchase behavior

Participants in Survey 1 received a brief introduction to CCU-based bioplastic bottles as a preference for the survey. Table 3 demonstrates the current behaviors of the survey respondents with respect to water bottle usage. Approximately half of the respondents habitually bring their own reusable water bottles when they are away from home. However, around 7% of participants do not have their own reusable water bottle. For the water bottle materials, the stainless steel and plastic reusable water bottles are the top two selections. Around 50% and 29% of respondents have chosen stainless steel water bottles and plastic water bottles, respectively. Nevertheless, 0.88% of participants only considered the single-use plastic bottle. Most of the respondents have never used single plastic bottles because they use their own reusable water bottles, but the maximum count of single plastic bottles used on average per week is 98, and the mean value is 5 (*Std. Deviation*: 13.4).

Respondents were asked to self-identify their level of knowledge about bioplastic bottles. Approximately half of the participants have heard about bioplastic bottles but cannot explain what it is and can describe a little bit. Around 28% have never heard of bioplastic bottles due to the emergence of products for environmental benefits. Only 1 person indicated having heard about it and is capable of providing a comprehensive explanation within the appropriate context. When survey participants were asked about the type of bioplastic, the response of 29.11% of those surveyed indicated that they only knew bioplastic generally. A total of 10.76%, 17.09%, 6.33%, 4.3%, and 11.39% of participants have known starch-based, cellulose-based, proteinbased bioplastics, aliphatic polyesters, and organic polyethylene, respectively. However, around 20% of them are unaware of any of the bioplastic types mentioned above.

In order to understand the reasons that prevent respondents from buying or using bioplastic bottles, options are included as follows: health/safety concerns, lack of information about the products, limited awareness, limited availability, design, low quality, high cost, recycling issues, not available where they live, and others. The results of this question demonstrated that 19.49% of respondents refrained from purchasing bioplastic bottles due to insufficient information about the products. The factors influenced participants who do not buy bioplastic bottles in the following order: limited availability (18.64%), limited awareness (19.49%), not available where I live (13.56%), high cost (10.17%), others (7.20%), health/safety issue (5.51%), recycling issue (4.24%), low quality (2.54%), and design (1.27%). The dominant reason for respondents who chose the “other” option is they already own their reusable water bottles and would not consider plastic bottles. The number of survey respondents (40.71%) who indicated that they somewhat agree the environmental impact of the bioplastic bottles impacts their decision to purchase this product. A total of 24.78% strongly agree that environmental impact is the main factor to change their decision, with 20.35% of participants in neutral status.

Figure 13 represents the price that respondents are willing to pay more or less for the single-use CO_2-based bioplastic bottles. Overall, approximately 41% of respondents indicated that they were willing to pay 25% more to buy single-use bioplastic bottles than conventional single-use plastic bottles, whereas 9.73% would pay 75% more, 11.5% would pay 100% more, and 1.77% would willing to pay 200% more. A total of 23.01% would buy bioplastic bottles at the same price as conventional plastic bottles. However, 7.08% and 0.88% would pay 25% and 100% (free) less. 5.31% of respondents would not consider this product because it is a “single-use” bioplastic bottle. This finding shows most of the participants are willing to pay more to buy products that have environmental benefits. Besides, as shown in Figure 14, the percentages for a series of categories represented varying levels of price of bioplastic bottles compared to conventional water bottles from the supported survey. Based on the results, the majority of participants (26.2%) are willing to pay $1 more to purchase the sustainable product, with 11.9% considering the alternative product if priced the same as the conventional one. Meanwhile, 23.8% would not purchase any plastic water bottles at any price. The follow-up survey has similar results to the first one. Few respondents are interested in buying the bioplastic alternative at a lower price, while the majority are willing to pay more for sustainable water bottles.

Ten crucial factors that influence respondents to decide to purchase bioplastic bottles include price, durability, composability, biodegradability, recyclability, reusability, raw materials, aesthetics, environmental footprint, and others. The response of 19.52% of those surveyed indicated that the price is the most significant factor affecting them to buy the single-use bioplastic bottles. Around 14% of respondents think recyclability and environmental footprint are factors that impact their decision. Table 4 explains the ranking of these ten factors for their decision. Price is the primary preference among respondents (52.21%), while 6.19% ranked price as their second preference. 18.58% and 21.24% of participants ranked durability as 1 and 2, respectively. Composability was ranked as the 3rd preference, with 6.19% of respondents ranking it as 1 and 15.93% ranking it as 2.

Table 3. Results on consumer usage and awareness of reusable and bioplastic water bottles.

Questions	**%**

Q8. How often do you bring your own reusable water bottle when you are away from home?		
	Never (0 day/week)	7.08
	Rarely (1-2 days/week)	13.27
	Sometimes (3-4 days/week)	12.39
	Very often (5-6 days/week)	16.81
	Everyday (7 days/week)	50.44
Q9. What type of reusable water bottle do you currently use?		
	Plastic	29.20
	Aluminum	8.85
	Stainless steel	50.44
	Glass	8.85
	Other	1.77
	I only use single-use plastic bottles	0.88
Q11. Have you heard of bioplastic bottles in general?	Never heard of it	28.32

	Heard about this but I would not be able to explain what it is really about	25.66
	Heard about this and could probably describe them a little bit	37.17
	Heard of it and familiar with this and I would be able to explain this well	7.96
	I'm very familiar with this and I can explain everything in context	0.88
Q14. How do you feel about this statement: "The environmental impact of the bioplastic bottle factors into my decision to purchase this product."	Strongly disagree	1.77
	Somewhat disagree	12.29
	Neutral	20.35
	Somewhat agree	40.71
	Strongly agree	24.79

Table 4. Consumer rankings of product attributes. Labeled 1,2, and 3 represent the rankings from the most to least important attributes influencing consumers' decision to purchase single-use CO_2-based bioplastic bottles.

%	Ranking		
	1	2	3
Price	52.21	6.19	1.77
Durability	18.58	21.24	7.96
Composability	6.19	15.93	15.04
Biodegradability	2.65	15.93	14.16
Recyclable	4.42	15.04	16.81
Reusability	2.65	4.42	17.70
Raw materials	5.31	8.85	10.62
Aesthetic	3.54	9.73	8.85
Environmental footprint	2.65	1.77	7.08
Other	1.77	7.69	0

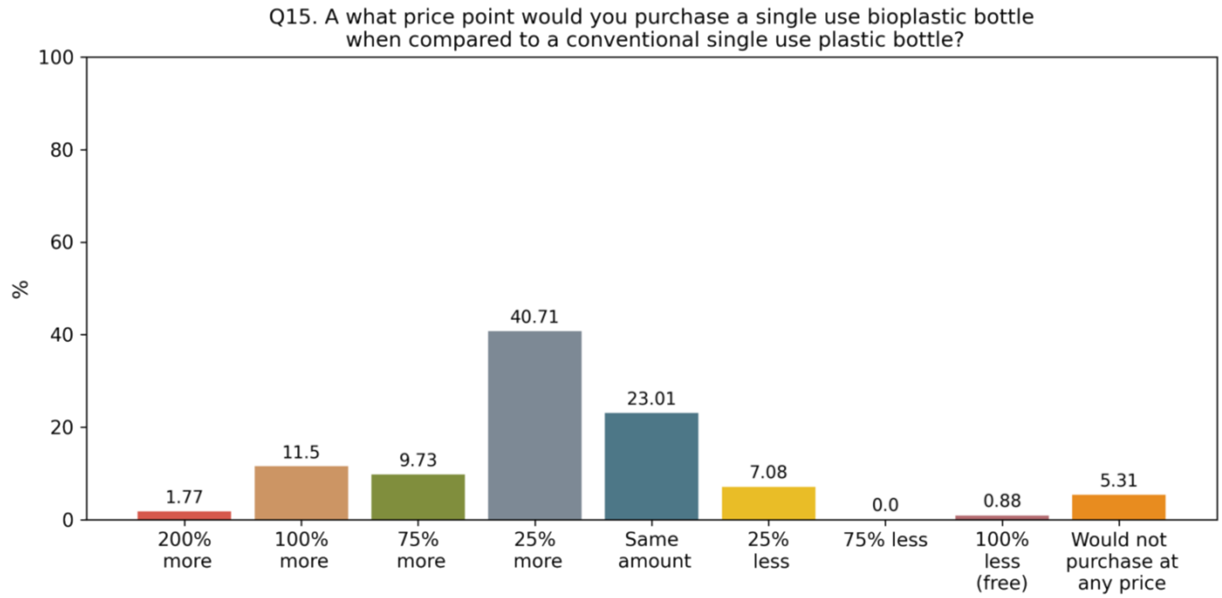

Figure 16. Distribution of price willing to buy bioplastic bottles compared to conventional ones from Survey 1.

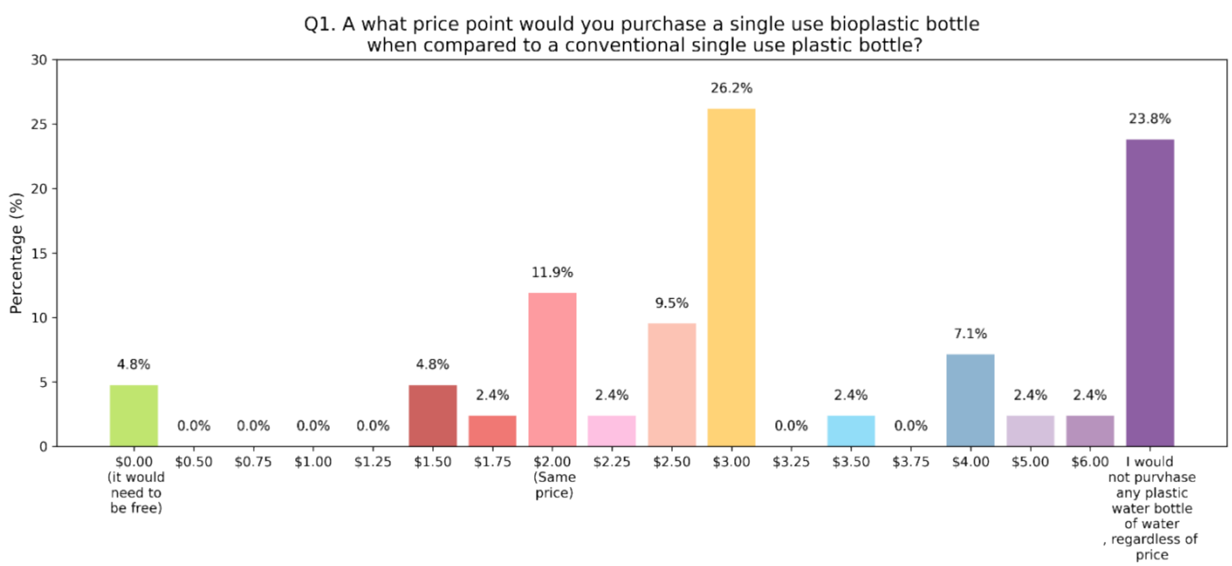

Figure 17. Distribution of price willing to buy bioplastic bottles compared to conventional ones from Survey 2.

4.5. Discussion

The two sets of WTP results from the surveys provide crucial insights into consumer behavior regarding sustainable products, specifically carbon-captured single-use bioplastic water bottles. These results indicate that more than half of the participants are willing to pay more to support sustainable alternatives beyond conventional options, reflecting a positive shift towards sustainability in consumer purchasing preference. The findings from this research were consistence with those of previous studies (De Marchi et al., 2020; Skouloudis et al., 2023; Zwicker et al., 2023).

A growing awareness among consumers of the environmental impact associated with traditional plastic production and disposal is presented in this study. This awareness influenced consumers' WTP for alternatives that have a lower environmental footprint, even if it means paying a premium. Participants' WTP more for bioplastic water bottles indicates that consumers are not only aware of environmental issues but are also prepared to act on this knowledge by choosing products that are less harmful to the environment. Besides, the WTP results emphasize the potential market viability for new bioplastic products. Companies and investors considering the production and commercialization of bioplastics may interpret these findings as a positive indication that there is a market segment which significantly values sustainability. This could encourage more companies to explore and expand their range of sustainable novel products, knowing there is a consumer base that supports such initiatives. Furthermore, the difference in WTP between the two surveys might reflect various demographic or psychographic factors influencing consumer decisions, such as income levels, environmental consciousness, or exposure to information about the benefits of bioplastics. For example, the environmental consciousness or environmentalist identity of participants has a significant connection with the WTP of bioplastic water bottles, which corresponds with previous research findings (Zwicker et al., 2023). Understanding these underlying factors can help marketers and policymakers design targeted strategies to promote broader adoption of sustainable products.

These WTP results highlight the importance of continuing to educate the public about the benefits of sustainable alternatives. They also determine the need for policies that support the development and adoption of such technologies, potentially through subsidies, tax incentives, or regulations that prefer environmentally friendly products over traditional plastics.

Limitations are of course present in all studies, particularly in small-scale surveys. First, the sample size for both surveys 1 and 2 are relatively small. Which means that it may not be representative of the overall population across the US. Second, both survey endeavors include a convenience sample, which may also cause the data collected not to be generalizable. In survey 1, many of the respondents were college or university students, who often skew towards being more environmentally conscious than the average American. Furthermore, Survey 1 is distributed via the internet and needs to be filled out online. The older may not be able to fill out the survey or do not have the opportunity to know this survey because they are unfamiliar with using the internet.

Although the limitations of this work are significant, it also represents one of the first US-based attempts to quantify the WTP of consumers for bio-based plastics. The authors sincerely hope that future work will be able to build on the work presented here.

4.6. Conclusion

The results of the survey were conducted on attitudes toward the adoption and WTP for CO_2based single-use bioplastic bottles in the USA. The findings indicate that there is consumer demand for sustainable materials, as attitudes were positive and the potential willingness to pay more for CO_2-based bioplastic bottles compared to conventional fossil-based ones. These outcomes, in conjunction with other factors such as environmental consciousness and sociodemographics, demonstrate that there is a demand for more sustainable options and consumers might be willing to pay a higher initial cost for alternatives. The results also provide insights into the possible marketing strategies for bioplastic products.

4.7. Acknowledgement

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5. Potential of Single-use CO_2-based Bioplastic Water Bottle Adoption Using Agent-based Modeling

The following chapter has been submitted for consideration for publication with the citation:

Feng, D., Hicks, A.L., Potential of Single-use CO2-based Bioplastic Water Bottle Adoption Using Agent-based Modeling.

The article appears as submitted, although style and formatting modifications have been made.

Authorship contribution statement

Danyi Feng: Designed Research, Performed Research, Analyzed Data, Wrote the Paper.

Andrea Hicks: Designed Research, Revised the Paper.

5.1. Abstract

Single-use plastic water bottles are ubiquitous in daily life. Most commonly these bottles are made from petroleum-based plastics, in particular polyethylene terephthalate (PET). However, conventional plastic water bottles result in substantial environmental pollution and plastic waste. Innovative technologies that utilize captured carbon as raw materials for producing bioplastic water bottles offer the potential to mitigate at least some environmental impacts. Understanding the factors that influence consumer adoption of sustainable alternatives is essential. This study utilizes Agent Based Modeling (ABM) to investigate the adoption dynamics of bioplastic water bottles, analyzing the influence of individual behaviors and social interactions within consumer

networks. The findings demonstrate that the cost is a significant factor influencing the adoption rate, while environmental benefits motivate some consumers to select bioplastic water bottles over conventional ones. Moreover, the results emphasize the importance of social networks, indicating that close connections among consumers lead to quicker and more widespread adoption due to peer influence.

5.2. Introduction

Plastic is a petroleum-based material that is widely used for food and beverage packaging, and ubiquitous due to its versatility, moldability, ability to be heat-sealed, ease of printing, and low cost of production (Filho et al., 2022; Kan and Miller, 2022). Single-use plastic bottles, such as those used for the storage and sale of bottled water are widely available.Several types of plastic are currently used for drinking water bottle production, including polyethylene terephthalate (PET), high-density polyethylene (HDPE), and polycarbonate (PC) (Filho et al., 2022; Yun et al., 2018). PET dominates the polymer market which is primarily used in the production of packaging materials, especially drinking water bottles (Benyathiar et al., 2022; Di Bartolo et al., 2021). In 2021, 44.7% of single-use beverage bottles were produced from PET compared to 3.4% from HDPE in the United States (Benyathiar et al., 2022). However, petroleum-based plastic water bottles pose significant risks to the environment due to upstream raw materials and manufacturing burdens and downstream plastic waste(Murugan et al., 2020). For water bottle production, 4% of global crude oil production was intended for use in 2016 (Murugan et al., 2020), and this led to large correspondingly carbon emissions (Papong et al., 2014). One pressing issue with respect to conventional petroleum-based plastic is that it is non-biodegradable, and results in the production of plastic waste and contaminants (e.g., microplastics). Microplastics in particular are a recent area of concern, remaining in the soil and ocean for the long periods of time and accumulating in land areas (Bakar and Mohamed, 2024; Zhang et al., 2021). Therefore, sustainable alternative materials are necessary for substitution to prevent and reduce environmental pollution.

The term bioplastics have been used loosely to categorize both biobased plastics, those are plastics sourced from biobased feedstocks, and biodegradable plastics those which degrade in the environment (Morris and Hicks, 2022b). Biobased plastic is non-biodegradable and produced from biological sources, such as polyethylene furanoate (PEF). Biodegradable plastic is made from conventional fossil sources but has intrinsic biodegradable properties due to additional chemical additives, such as polycaprolactone (PCL). Biobased and biodegradable plastics are made from biomass and have biodegradable characteristics, such as polylactic acid (PLA). In order to reduce carbon emissions and threats to the ecosystem, biobased and biodegradable polymers are considered the best option to replace conventional plastics (Tamburini et al., 2021). Currently, the most common carbon feedstock for bioplastic (biobased and biodegradable) production are plant-based sources (Di Bartolo et al., 2021), such as potato starch, glycerol, and sunflower meal from sunflower oil production (Atiwesh et al., 2021c; Dietrich et al., 2020; Manali Shah et al., 2021). Nevertheless, other carbon sources can be potentially used for bioplastic manufacturing, such as captured carbon dioxide (CO_2) (McAdam et al., 2020). Therefore, bioplastic produced from captured CO_2 is a potentially sustainable plastic alternative to achieve the goal of carbon utilization from greenhouse gas emissions.

Globally, approximately one million plastic water bottles are purchased every minute (Laville and Taylor, 2017). In the United States, beverage packaging unit sales totaled $195 million in 2013 (Kang et al., 2017), and annual consumption per capita of single-use plastic water bottles was reported at 50 billion units (Bruchmann et al., 2021). Due to the alarming environmental and human health consequences of single-use petroleum-based plastic water bottles, an increasing number of bioplastic alternatives have been purchased by commsumers currently (Notaro et al., 2022b). The most common bioplastics are available for consumer products including PLA, PCL, and bioderived polyethylene (Bio-PE) (L. Dilkes-Hoffman et al., 2019). Understanding the factors that influence consumer selection for bioplastic alternatives is necessary. However, it is complicated to model human decision-making for a technological transition from conventional plastic water bottles to bioplastic water bottles. Overall, consumer preferences are significantly influenced by environmental concerns, particularly CO_2 emission reductions. Scherer et al. (2018) highlighted a strong preference for bio-based products in Germany, like water bottles and running shoes made from various international crops, particularly at lower price points. This suggests that while consumers are environmentally conscious, their purchasing decisions remain sensitive to price. De Marchi et al., (2020) found that consumers in Italy were willing to pay a premium for bioplastic water bottles over those made from conventional plastics when provided with sustainability information, indicating that informed consumers may value environmental benefits sufficiently to incur higher costs. Similarly, in Greece, a significant portion of respondents expressed willingness to pay more for innovative bioplastic products, suggesting a trend towards environmental responsibility among consumers (Skouloudis et al., 2023). These findings illustrate that consumers are inclined towards sustainable products, especially when these products are competitively priced and when consumers are well-informed about the environmental benefits.

The adoption of new consumer products, is not straightforward to model. There are various approaches available for simulating the behavior of complex systems, including system dynamics and agent-based modeling (ABM). System dynamics uses a top-down approach, focusing on aggregate behavior and feedback loops across the whole system, and is suited for studying broad trends over time (Horvat et al., 2018; Wang et al., 2014). ABM, on the other hand, takes a bottom-up approach, modeling individual agents and their interactions to understand emergent phenomena, making it ideal for systems where details at the micro-level significantly impact outcomes (Hicks and Theis, 2014; Wang et al., 2014; Zhang et al., 2011). Regarding the adoption of sustainable water bottles by consumers, which is primarily an individual choice affected by numerous factors, applying an ABM approach is an appropriate methodology to employ.

This paper utilizes ABM with the multicriteria evaluations of single-use water bottle options to simulate the adoption of single-use carbon captured bioplastic water bottles compared with conventional water bottles in the United States. The purpose of this study is to better understand adoption behaviors and the potential for policy interventions.

5.3. Methods

ABM is used to investigate the factors that influence the decisions by agents to choose two single-use plastic water bottles: CO_2-based bioplastic water bottles and conventional water bottles (e.g., polyethylene terephthalate (PET)).

Cellular automata (CA) are a typical ABM method that simulates the behavior of systems composed of multiple interconnected components (Hicks and Theis, 2014; Kowalska-Styczeń, 2017). This modeling technique, first conceptualized by John von Neumann and Stanislaw Ulam in the 1940s, is used extensively to understand complex, dynamic systems across various disciplines, including physics, biology, and social science (Wolfram, 1983)(Wolfram, 1983). In the area of social science, CA has been particularly effective in analyzing how individual behaviors can lead to complex group dynamics and emergent phenomena (Schelling, 1971). In CA, the state of each cell in the grid is determined by the states of its neighboring cells and repeatedly changes over time (Wolfram, 1983). This approach provides valuable insights into the mechanisms driving human behavior and social change (Gilbert and Troitzsch, 2005).

This study utilized the ABM model composed of a 625-agent grid (25 by 25 agents), where each agent represents a customer seeking to purchase either a single-use bioplastic or single-use conventional water bottle. In the CA method used, agents select their preferred single-use water bottles by maximizing their personal utility function. All water bottle options are modeled as standard 20 fluid ounce (591 mL) bottles, interchangeable in size and function, reflecting the current market choices between bioplastic and conventional plastic. The specific starting characteristics used for single-use plastic water bottles are a conventional option (price - \$1.5 (Optimum Water Solutions, 2022), compostability - 450 years (Hossain and Tuha, 2020), biodegradability - 10 years (Koller and Mukherjee, 2022), environmental footprint - 0.134 kg CO_2 eq/bottle (Tamburini et al., 2021), and a bioplastic option (price - \$3.69 (Cabrey, 2022), compostability - 0.5 years (Koller and Mukherjee, 2022), biodegradability - 1.5 years (L. S.

Dilkes-Hoffman et al., 2019; Koller and Mukherjee, 2022), environmental footprint - 0.177 kg CO_2 eq/bottle (IBWA, n.d.; Koch et al., 2023). The initial selection of water bottle raw materials, price to purchase product, and agent typologies were determined by using survey data from the USA. Agent typologies are presented in Table 1 and are based on the relative importance of nine identified factors influencing the selection of new plastic water bottles using survey data (presented in Appendix D).

In Table 5, agents are categorized based on the factors they identified as most significant. The common characteristics of the majority of agents in each group were applied to the entire group. Type 1 is the largest group, representing 52.21% (326) of agents who identified price as the most important reason to adopt CO_2-based bioplastic water bottles. Besides, the second largest group is type 9, which means 21.24% of those considered environmental footprint as the most important factor to affect their bioplastic water bottle adoption decision-making. Unsurprisingly, only a few participants (0.88%) indicated aesthetics (type 8) as the most important reason to adopt single-use bioplastic water bottles. The rankings of each typology are utilized to assign weights in the utility function equation for two water bottle options.

Table 5. Agent typologies based on survey data (1 = most important, 9 = least important).

Typology	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
% of agents	52.21	3.19	1.77	6.19	1.77	3.54	3.54	0.88	21.24
Price	1	2	9	2	9	2	2	3	2
Durability	2	1	7	5	3	3	5	4	7
Compostability	3	8	1	2	6	5	2	8	5
Biodegradability	4	5	4	1	7	4	4	7	3

Recyclability	5	7	5	3	1	6	6	5	3
Reusability	6	3	8	7	4	1	7	6	7
Raw materials	7	4	3	8	5	7	1	2	8
Aesthetics	8	9	6	9	3	8	9	1	9
Environmental footprint	9	4	2	4	9	9	8	9	1

Figure 15 demonstrates the process by which each agent makes a decision for the type of water bottle adoption at the "purchase opportunity moment". When agents consider buying the water bottles, they will evaluate the total utility of all two water bottle options. A linear utility function is employed to evaluate the benefits, where each agent evaluates the utility of plastic bottle types ($U_{plastic\ bottle}$) based on the characteristics of factors (C_1 through C_n) of the option weighted by the importance of each factor to the agent when selecting plastic bottle types (w_1 through w_n):

$$U_{plastic\ bottle} = C_1w_1 + C_2w_2 + \cdots + C_nw_n \qquad \text{Equation 7}$$

where $U_{plastic\ bottle}$ is the utility function of bioplastic or conventional water bottles, C represents the physical characteristics (e.g., cost, durability, environmental footprint, etc.), and w is the weighting score of the nine typologies. Characteristic factors and weighting scores are scaled between 0 to 1 to prevent the numerical dominance of a single factor.

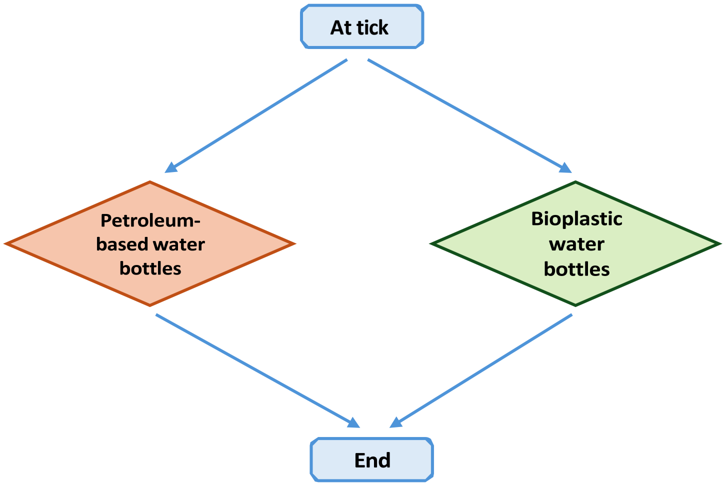

Figure 18. Flow chart of agents' decisions per turn, each turn represents 1 week and a total of 5 years (260 weeks).

The probability of the agent adopting the particular bioplastic bottle technology is defined by the utility (equation 8):

$$P_{bio} = \frac{U_{biop}}{U_{bio} + U_{conv}} \qquad \text{Equation 8}$$

where the probability of bioplastic bottle adoption (P_{bio}) is the utility of the bioplastic option divided by the summation of the utility of bioplastic and conventional water bottles (U_{bio}, U_{conv}).

$$P_{conv} = 1 - P_{bio} \qquad \text{Equation 9}$$

where the probability of conventional option adoption (P_{conv}) is 1 (overall probability of selection) subtracted from the probability of a bioplastic option. The roulette wheel simulation method is used to select the single-use water bottle adoption (Hicks et al., 2015). The reason for utilizing utility to determine the probability of adopting water bottles, rather than choosing the water bottle type with the highest utility, is to acknowledge factors excluded in the model that could have unknown impacts or an individual might select a bottle with lower utility even probability is small (Hicks et al., 2015b). This probabilistic approach is intended to encompass such uncertainties.

Table 6 presented twenty different scenarios that were simulated. These scenarios contain the various potential situations that may influence the decision-making for single-use water bottle adoption options. The scenarios consider potential changes to the price and environmental impact of bioplastic water bottles, typologies, and neighbors' influence on adoption decision-making. Scenarios 1 – 3 seek to understand the influence of neighbors on agents for new product adoption decision-making. Scenarios 4 – 7 assume that the price of bioplastic water bottles is the same as, 0.75 times, 0.5 times, and free compared to conventional water bottles, respectively. Similarly, scenarios 8 – 15 assume that the carbon emission of bioplastic water bottles is 2 times, 1.5 times, 1.25 times, same as, 0.75 times, 0.5 times, 0.25 times, and no emission compared to the conventional one, respectively. Scenarios 16 – 24 are considered the variation of bioplastic water bottle adoption when the typology is consistent. This model runs each week for 5 years, a total of 260 weeks. It is assumed that each week when an agent goes to purchase a single-use bottle they will calculate the utility of the choice. This is synonymous with someone purchasing a weekly single-use bottle of water.

Table 6. Scenarios for simulation.

Scenario Numbers	**Scenarios**	**Scenario description**
	Neighbors influence	

1	No neighbors	Neighbors do not have any influence on the adoption
2	4 neighbors	The adoption decision will be affected by the 4 neighbors around the agent
3	8 neighbors	The adoption decision will be affected by the 8 neighbors around the agent
	Cost	
4	Same cost	The bioplastic and conventional water bottles cost the same
5	0.75 cost	The bioplastic water bottle is ¾ the price of the conventional one
6	0.5 cost	The bioplastic water bottle is ½ the price of the conventional one
7	Bio free	The bioplastic water bottle is free
	Environmental footprint (EF)	
8	2 EF	Bio EF is 2 times conventional EF
9	1.5 EF	Bio EF is 1.5 times conventional EF
10	1.25 EF	Bio EF is 1.25 times conventional EF
11	Same EF	EF is the same for both types of water bottles
12	0.75 EF	Bio EF is ¾ of conventional EF
13	0.5 EF	Bio EF is ½ of conventional EF
14	0.25 EF	Bio EF is ¼ of conventional EF
15	No bio EF	Bio EF is free
	Agent consideration	
16	All type 1 (price)	All agents are type 1, with 4 neighbors
17	All type 2 (durability)	All agents are type 2, with 4 neighbors
18	All type 3 (compostability)	All agents are type 3, with 4 neighbors
19	All type 4 (biodegradability)	All agents are type 4, with 4 neighbors
20	All type 5 (recyclability)	All agents are type 5, with 4 neighbors
21	All type 6 (reusability)	All agents are type 6, with 4 neighbors
22	All type 7 (raw materials)	All agents are type 7, with 4 neighbors
23	All type 8 (aesthetics)	All agents are type 8, with 4 neighbors
24	All type 9 (EF)	All agents are type 9, with 4 neighbors

5.4. Results

The average cumulative number of bioplastic and conventional water bottle adoptions, associated with the differences and standard deviations under various neighbors' influence scenarios, are presented in Table D1. Overall, the agents are willing to adopt more bioplastic water bottles than conventional ones. Comparing these three scenarios, the results show a slight variation in adoption rates for both types of bottles as the number of neighbors changes but the differences are minimal. Specifically, the adoption rate of bioplastic water bottles slightly decreases as the number of neighbors increases, from no neighbors to 8 neighbors. Conversely, for conventional water bottles, the adoption rate increases as the number of neighbors grows. The standard deviations indicate variability in adoption rates, and the higher variability is observed with 8 neighbors at 52.74 for bioplastic bottles compared to no neighbors and 38.52 when compared to four neighbors at the end of the simulation period. This suggests less consistency in behavior as the number of neighbors increases. The results demonstrate that increased social interactions or visibility among more neighbors could influence individual decisions, leading to a decrease in bioplastic bottle adoption as the neighborhood network increases.

As shown in Figure 16, the cumulative adoption of bioplastic water bottles over 260 weeks (5 years) depends on 4 neighbors and is segmented by different pricing strategies relative to conventional bottles. The trends demonstrate the total number of bioplastic bottle adoption rates are highest when the bottles are offered for free. When the cost is reduced to half of conventional bottles, adoption remains robust but slightly less than the free option. As the price increases to 75% of the conventional cost, the adoption rate slows further, and it is least likely for agents to adopt when the bioplastic bottles are priced the same as conventional bottles. This pattern underscores the significant role that pricing plays in consumer acceptance and the transition to environmentally friendly alternatives, with lower costs driving higher bioplastic adoption. This figure presents only the adoption rate of bioplastic water bottles because the total number of bottles adopted each week remains constant, and any increase in bioplastic adoption corresponds to a decrease in conventional plastic adoption.

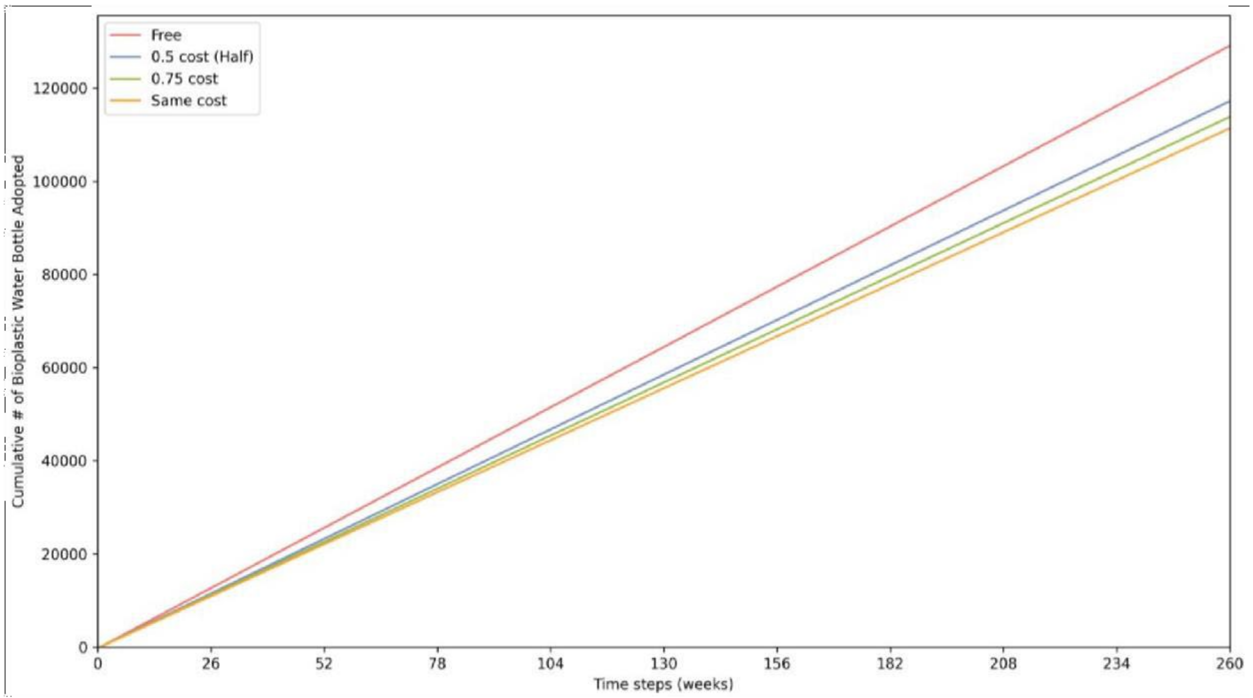

Figure 19. The average cumulative adoption trends of bioplastic water bottle cost changes over 5 years.

Figure 17 presents the cumulative adoption of bioplastic water bottles over 5 years, differentiated by environmental footprint based on 4 neighbors. The highest adoption rates are seen with bioplastic bottles having no EF, emphasizing that lower environmental impacts encourage more rapid consumer uptake. As the EF increases, the adoption rates gradually decline, indicating that consumers are less inclined to choose options with higher environmental costs relative to that of the conventional plastic bottle. This result shows a distinct consumer preference for products that minimize environmental impacts, although a significant number of consumers continue to select options with higher footprints, which is possibly influenced by factors like product availability, brand loyalty, or lack of alternatives. These trends highlight the importance of environmental considerations in consumer decision making, particularly in the context of sustainable products.

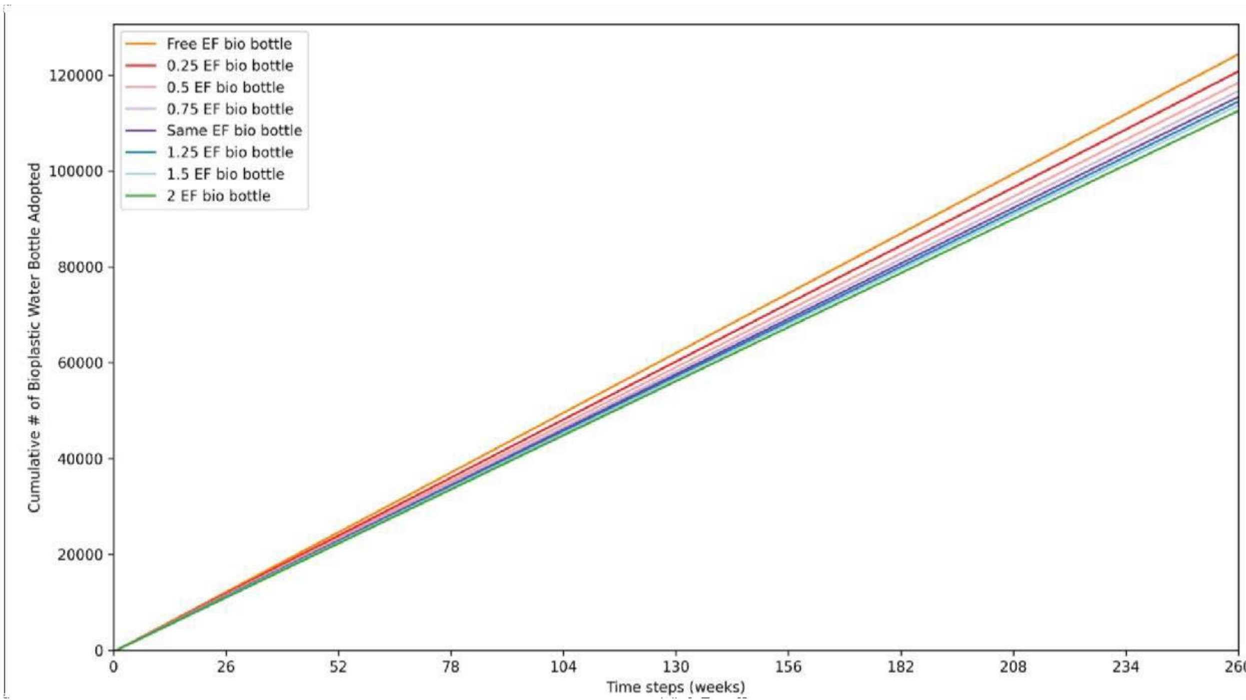

Figure 20. The average cumulative adoption trends of various environmental footprint scenarios for bioplastic water bottles over 5 years.

The cumulative adoption of water bottles over a period of 5 years, categorized by nine different typologies from type 1 to type 9, is illustrated in Figure 18. Each line represents the adoption path of a specific typology over time. The adoption rates for all typologies show a steady increase, suggesting consistent growth in the uptake of bioplastic water bottles. This occurs regardless of typology because the total number of water bottles purchased each turn remains constant. However, there are slight variations in the slope of each line, indicating that some typologies are adopted more quickly than others. For instance, if the agents are all type 2 (compostability) and type 7 (raw materials), the adoption rate of bioplastic bottles is highest, rising more sharply compared to others such as all type 9 (EF) which has a relatively flatter slope.

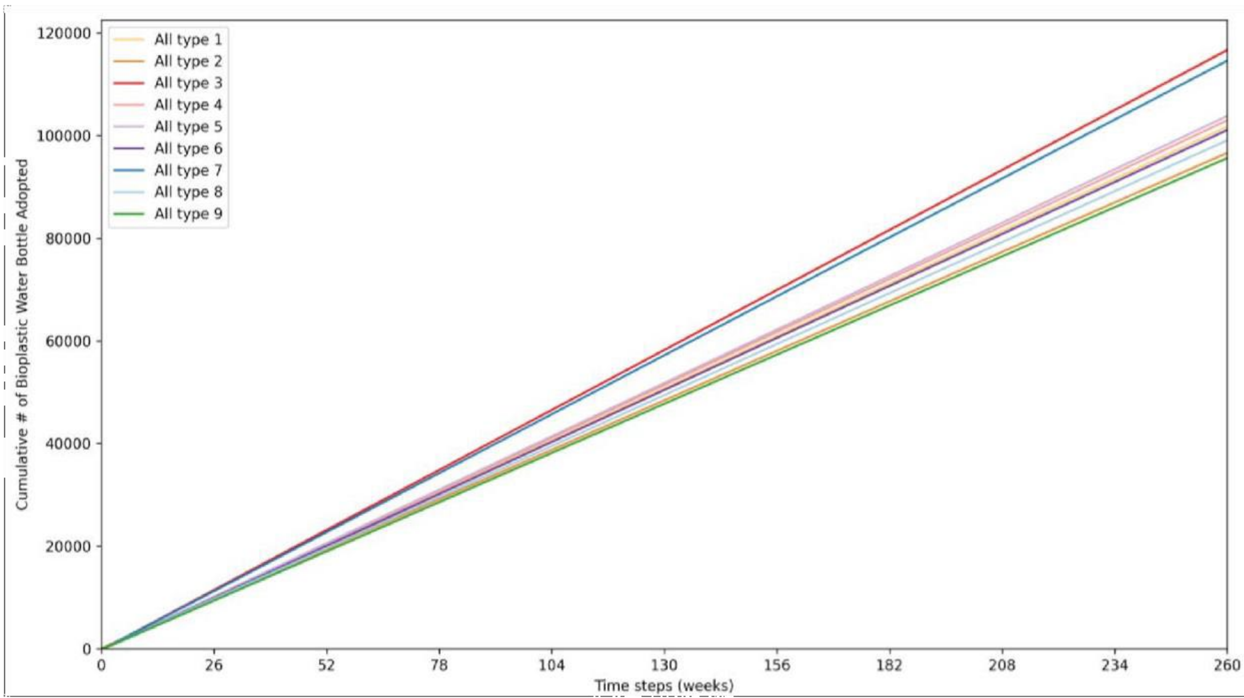

Figure 21. The average cumulative adoption trends of various typology scenarios for bioplastic water bottles over 5 years.

Figure 19 shows the trends where cost and EF together influence the adoption of bioplastic bottles over 5 years (260 weeks) using 4 neighbors as the baseline. Each line represents a unique combination, highlighting how both pricing and environmental impact affect consumer adoption rates: (1) free cost and EF of bio represent bottles that are both free in price and EF; (2) free cost and 0.5 EF mean bottle are free with a half environmental impacts of typical water bottles; (3) free cost and same EF scenario is that bio bottles are free but have same EF as conventional one; (4) free cost and 2 EF describe the free bio bottles with a footprint twice; (5) same cost and EF give the price and EF of bio one as same with convention one; (6) same cost and free EF prices the same but with no EF of bio one compared to conventional one; (7) same cost and 2 EF of bio scenario has same cost but with a footprint double of conventional bottles. The findings suggest free bottles, regardless of their environmental footprint, generally see higher adoption rates, illustrating the strong effect of cost elimination on consumer behavior. Conversely, bioplastic bottles that carry the same cost as typical conventional ones, even those with better environmental attributes, are adopted more slowly, indicating that cost remains a significant barrier despite environmental benefits. This result highlights the complex interaction between cost-effectiveness and environmental sustainability in consumer choices.

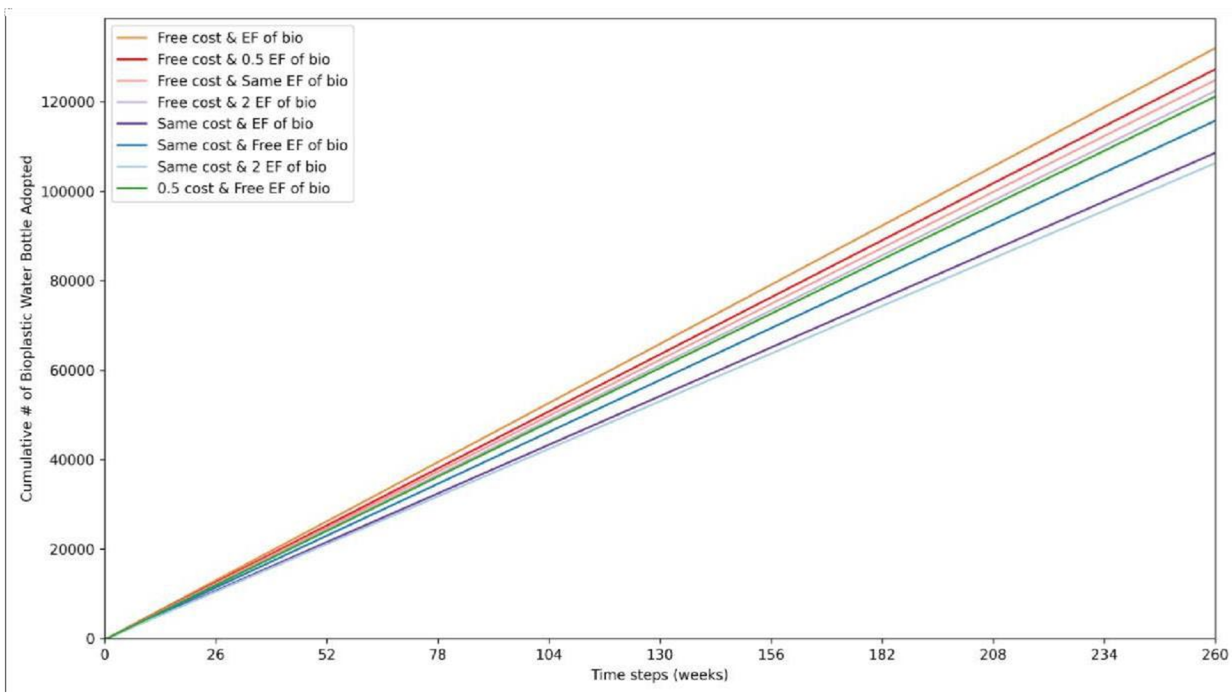

Figure 22. The average cumulative adoption of bioplastic water bottles over 260 weeks by cost and EF combinations.

The results from Table 7 and Table D2 explain the influence of the weighting of neighbors' change (W10) on the cumulative adoption of bioplastic water bottles, considering two different neighborhood sizes: 4 and 8 neighbors. For both 4 and 8 neighbor scenarios, as W10 increases from 0 (no neighbor influence) to 1 (maximum neighbor influence), there is a noticeable increase in the average cumulative number of bioplastic water bottle adoptions. Specifically, the average cumulative adoption numbers start from approximately 100,509 and 100,518 for 4 and 8 neighbors respectively with W10 at 0, and progressively rise to 100,9422 and 100,9777 by the time W10 reaches 1. This trend indicates a positive correlation between the degree of neighbor influence and the rate of adoption, where a higher W10 value corresponds to more bioplastic water bottle adoption. When comparing the results between 4 and 8 neighbors, the increment of bioplastic adoption is more in scenarios with 8 neighbors. This demonstrates that more neighbors (denser social networks) may promote bioplastic water bottle adoption.

Table 7. The average value, differences, and standard deviation of weighting neighbors' importance changes based on 4 neighbors.

The weighting of neighbors’ change (W10)	Average cumulative # of bioplastic water bottle adoption (4 neighbors)	Standard deviation	95% confidence interval
0 (no neighbor)	100509.47	1.83	(384.73, 385.46)
0.1	100635.73	1.64	(385.25, 385.91)
0.2	100654.28	1.48	(385.35, 385.94)
0.3	100682.41	1.49	(385.46, 386.05)
0.4	100715.87	1.32	(385.62, 386.15)
0.5 (baseline)	100753.33	1.42	(385.76, 386.31)
0.6	100844.24	1.27	(386.12, 386.63)
0.7	100857.68	1.16	(386.20, 386.66)
0.8	100916.98	1.25	(386.41, 386.90)
0.9	100930.57	1.13	(386.48, 386.93)
1	100941.84	1.03	(386.54, 386.96)

5.5. Sensitivity analysis

A sensitivity analysis over 260 weeks, comparing the cumulative adoption of bioplastic bottles under various conditions with four neighbors as the baseline, is presented in Figure 20. Figure 20 (a) describes the trends when the cost of bio bottles increases to $100, and (b) gives the patterns when the EF of bio one is 100 times compared to conventional one. In both (a) and (b), the adoption curve for the baseline scenario consistently shows the highest trajectory, indicating that having 4 neighbors involved promotes the greatest adoption rate. The (a) demonstrates a significantly lower adoption rate in bioplastic bottles, suggesting that high costs are a major restraint to adoption. The (b) also shows reduced adoption compared to the baseline but not as substantially as the high cost scenario, indicating that while environmental impact is a consideration for consumers, the cost is a more critical barrier. This analysis emphasize the sensitivity of consumer behavior to both price and environmental impact, with price having a more significant effect on the adoption rates.

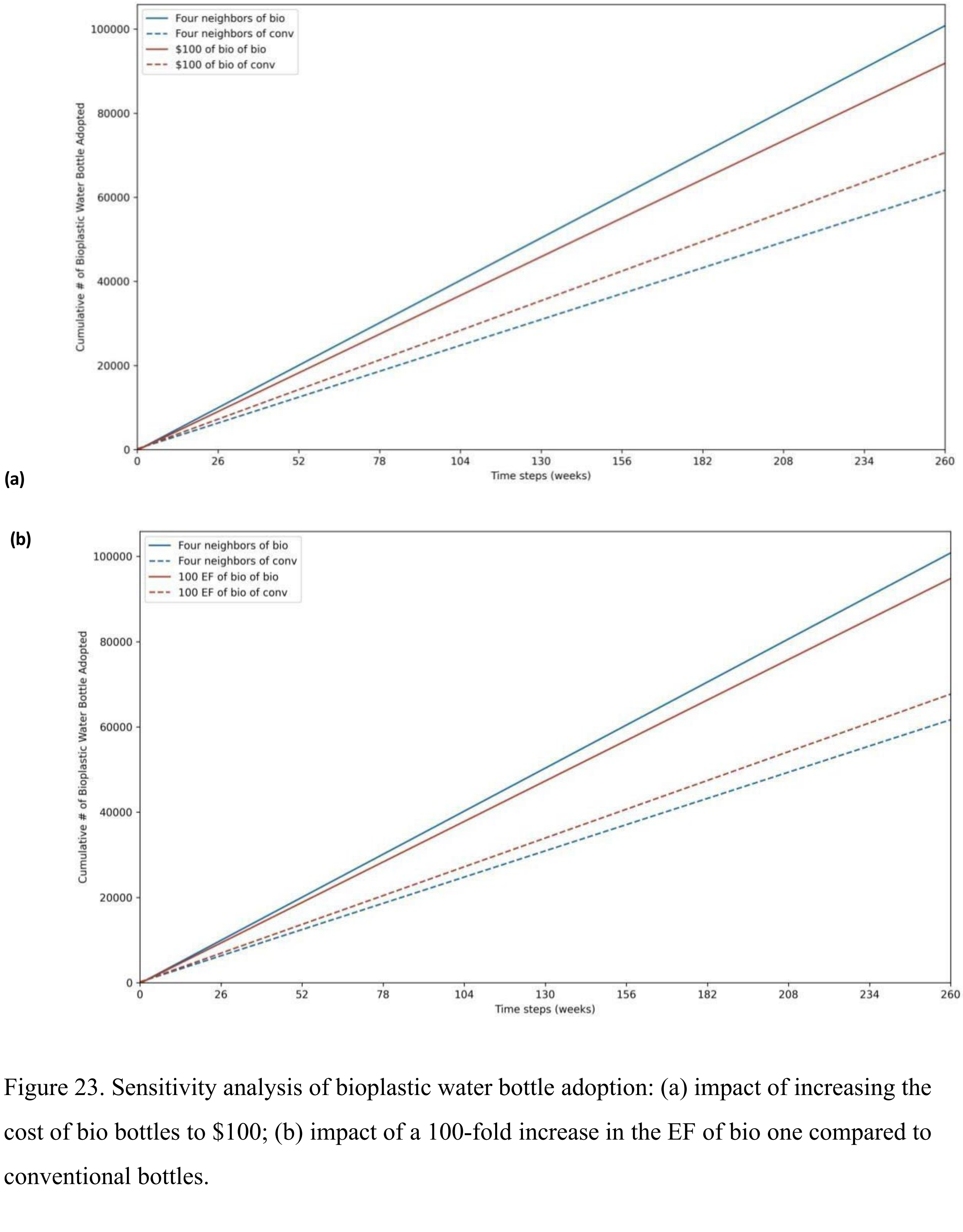

Figure 23. Sensitivity analysis of bioplastic water bottle adoption: (a) impact of increasing the cost of bio bottles to $100; (b) impact of a 100-fold increase in the EF of bio one compared to conventional bottles.

5.6. Discussion

This study presents a potential ABM of consumer adoption of a novel single-use water bottle compared to a conventional plastic single-use water bottle. It explains a complex interaction between various typologies and social dynamics in shaping consumer behavior towards singleuse CO_2-based bioplastic water bottles. The findings illustrate that the cost is a more decisive factor while neighbor influence and environmental considerations impact bioplastic water bottle adoption. This complex interaction between cost-effectiveness and environmental sustainability decides consumer preferences and emphasizes the need for strategic approaches to encourage the adoption of sustainable products.

The adoption of single-use bioplastic water bottles derived from captured CO_2 represents a promising solution to reduce the carbon footprint associated with traditional plastic production. When CO_2 is utilized as a raw material to produce bioplastics, not only is it prevented from contributing to atmospheric carbon levels, but it also substitutes for petroleum-based plastics which currently dominate the market. This switch has the potential to substantially decrease reliance on fossil fuels and mitigate carbon emissions. If bioplastic bottles were adopted on the same scale as conventional plastic bottles, it is estimated that more than 5.6 million metric tons of CO_2 could be sequestered annually per capita, dramatically illustrating the potential environmental benefits of this technology (Bruchmann et al., 2021; Koch et al., 2023). However, while the sequestration impact appears significant, a comprehensive life cycle assessment (LCA) study of polyhydroxyalkanoates (PHA) production provides concerns about environmental drawbacks throughout the product's life cycle. According to Koch et al. (2023), the production of

PHA using CO_2 as a raw material still has positive CO_2 eq emissions, due to the energy-intensive production processes. Therefore, if the energy sources are used from fossil fuels, the environmental benefits could be offset by carbon sequestration.

Moreover, increased CO_2-based bioplastic water bottle adoption could impact waste management systems, necessitating adjustments in recycling processes to accommodate bioplastics which may not be compatible with traditional recycling systems. For example, biodegradable bioplastic, such as PHA, requires different handling and processing for recycling compared to conventional plastic and may need separate collection and composting systems (Gioia et al., 2021). This is because the most common type of plastic (PET) is not compostable (Colijn et al., 2022). While the shift to more sustainable materials could initially result in challenges, such as contamination of recycling streams and additional adaptation costs, it may ultimately lead to more sustainable waste management practices. Additionally, estimating the environmental implications of bioplastic water bottles during their end-of-life phase is crucial for assessing their overall sustainability. Factors, such as biodegradability, recyclability, and the actual practices in waste management facilities, play a significant role in determining their environmental impact. For instance, if bioplastic bottles are designed to be compostable but end up in landfills where conditions are not conducive to biodegradation, they may not break down as intended and could contribute to methane emissions. Therefore, understanding the specific end-of-life pathways and ensuring that bioplastics are processed in environmentally beneficial ways are essential components of evaluating their effectiveness in reducing plastic pollution.

The results provide valuable guidance for developing more effective policy and market strategies aimed at increasing the adoption of sustainable products. For instance, if the results indicate that a cost reduction substantially increases the adoption of bioplastic bottles, policymakers could utilize this data to implement financial measures that encourage this trend. Besides, subsidies or tax incentives to manufacturers might be considered to reduce production costs, thereby enabling them to lower retail prices without compromising profitability.

5.7. Conclusions

This study determined significant insights into the factors influencing the adoption of single-use CO_2-based bioplastic water bottles. The results indicated the crucial influence of cost and EF in determining consumer preferences and adoption rates. Increasing agents are willing to adopt bioplastic water bottles at lower cost and/or less EF, whereas increased costs and greater EF tend to discourage consumers. Furthermore, this study emphasized the importance of neighborhood dynamics and how social factors can influence individual decisions regarding bioplastic usage. Increasing the degree of neighbor influence from no influence to maximum influence significantly enhances the cumulative adoption of bioplastic water bottles, with denser social networks showing an obvious effect on adoption rates. Moreover, the sensitivity analysis demonstrates the impact of extreme scenarios on adoption rates, reinforcing the need for balanced approaches that consider both economic feasibility and environmental benefits.

If adopted widely, this approach could sequester substantial CO_2 annually per person. However, a

LCA study indicated that the benefits could be compromised by the energy-intensive production processes, especially if powered by fossil fuels. Additionally, the integration of CO_2-based bioplastics into existing waste management systems poses challenges, necessitating new recycling protocols and systems to handle biodegradable options like PHA, which significantly differ from conventional plastics. Effective management of bioplastics' end-of-life phase is crucial to fully realize their potential in reducing plastic pollution, emphasizing the need for comprehensive strategies to ensure bioplastics contribute positively to sustainable waste practices. Subsidies or tax incentives for manufacturers may encourage the production of sustainable alternatives at lower costs, thereby reducing the sale price.

5.8. Acknowledgement

The author would like to thank all lab team members, and Han Liu for providing feedback on the manuscripts and figures.

6. Conclusions and future works

6.1. Summary and contributions

6.1.1. Summary

The first LCA paper (Chapter 2) presented significant gaps in research that were highlighted through a LCA derived from literature on enhanced weathering (EW) for 1 kg carbon sequestration, focusing on wollastonite for enhanced weathering. A comparative study between synthetic and natural wollastonite revealed that the natural form has a lesser impact on the environment and human health. Transitioning from natural to synthetic wollastonite showed more than a 100% increase in environmental and health impacts, although increasing production rates from 60% to 99% could reduce these impacts by 55%-68%. Ultimately, the findings suggest that using natural wollastonite for carbon capture is preferable, as synthesis proved less efficient and more harmful based on breakeven analysis results.

The second LCA paper (Chapter 3) provided cradle-to-gate impact assessment of 1 gram of PHB produced via electrochemical and biosynthesis processes. It was found that the electrochemical process is the primary contributor to environmental and human health impacts. Consequently, factors like the raw materials and technologies employed in the production of acetate, the length of the experiment, and the efficiency of the acetate produced can significantly affect environmental and human health outcomes. Although bioplastics use CO_2 as a raw material, the overall processes are not carbon-negative because of the energy-intensive manufacturing processes which often rely on fossil fuels, further contributing to the carbon footprint.

The third paper (Chapter 4) uses surveys to focus on U.S. consumer attitudes towards the adoption of CO_2-based single-use bioplastic bottles and their WTP compared to traditional fossilbased alternatives. The findings indicated a strong consumer interest in sustainable materials, with positive attitudes and a readiness to pay a premium for CO_2-based bioplastics. These outcomes, combined with factors like environmental awareness and socio-demographic influences, suggest a heavy demand for more sustainable product options, with consumers potentially willing to pay higher initial costs. Additionally, the results offer valuable guidance for potential marketing strategies for bioplastic products.

The fourth paper (Chapter 5) provided deep insights into the factors that affect the adoption of single-use CO_2-based bioplastic water bottles using ABM. It highlighted that both cost and environmental footprint (EF) play critical roles in affecting consumer preferences and adoption rates, with lower costs and reduced EFs enhancing adoption, while higher costs and larger EFs prevent it. Additionally, the study emphasized the significance of social dynamics within neighborhoods, showing that stronger social influences can significantly boost the overall adoption of bioplastic bottles, particularly in closely-knit social networks. The sensitivity analysis further illustrated how extreme scenarios could affect adoption rates, emphasizing the importance of strategies that balance economic and environmental considerations.

Overall, this series of LCA and ABM studies provided a comprehensive examination of the environmental impacts and customer behaviors for various sustainable technologies and consumer products. These papers contribute to the roadmap for future LCA, particularly those aiming to provide a holistic evaluation of both direct and indirect environmental impacts associated with social networks.

6.1.2. Contributions

When pursuing the goal of achieving net-zero GHG emissions through CCUS technologies, decision-makers face challenges of optimizing limited resources across various potential solutions. To make informed decisions on which CCUS technologies and projects to fund, a structured approach is essential, focusing on several key considerations. Technological maturity and scalability are factors that assess whether a technology is ready for widespread deployment and capable of being scaled to a level where it can significantly impact GHG reduction goals. Technologies vary in their development stages from laboratory scale to fully commercialized solutions. Mature technologies offer less risk and can provide immediate benefits, but emerging technologies may promise greater long-term advantages due to advancements in efficiency or effectiveness. Decision-makers should consider the technology readiness level and existing deployment examples to estimate maturity and scalability. Besides, evaluating cost-effectiveness involves not just looking at the upfront capital costs but also examining ongoing operational costs, maintenance expenses, and potential revenue streams from products derived from captured carbon. Technologies that can converse captured CO_2 into valuable products like concrete additives, fuels, bioplastics, or chemicals may offer a dual benefit of emissions reduction and economic return. A comprehensive cost-benefit analysis, including lifecycle cost assessments, can help identify the most economically viable options. The success of CCUS technologies often relate to a supportive regulatory environment. Technologies that align with current environmental regulations and can benefit from policy incentives such as carbon pricing, subsidies, or tax incentives are often more attractive. Decision-makers need to stay informed about both current policy circumstance and potential future changes to ensure the chosen technologies will remain viable and compliant over their operational lifespan. For social perspective, public perception can make or break the adoption of new technologies. Technologies that are viewed positively by the public are less likely to face resistance and more likely to receive community support. Effective engagement strategies, including transparent communication and community involvement in decision-making processes, can enhance public acceptance. Moreover, considering the social impact, such as job creation or impacts on local industries, is crucial in collecting community support. By thoroughly considering these detailed factors, decision-makers can strategically guide investments towards CCUS technologies that offer the greatest potential for achieving net-zero GHG emissions effectively and sustainably.

The CCUS technologies and products that I have evaluated are not appropriate to achieve the net-zero emission goal. For CCS study that using wollastonite to capture carbon emissions, the results indicate that the nature scenario has negative carbon emissions. However, the storage of nature wollastonite is not enough to be considered for carbon sequestration in a long-term period because there is not enough of it available. The synthetic scenario can continuously provide raw materials for enhanced weathering, but the emitted carbon emissions are higher than they captured. Therefore, both scenarios under current conditions are not recommended, but if the synthetic methods are still developed to reduce the emission from manufacturing processes and improve the efficiency of synthesis, the synthesized wollastonite can be considered to utilize for carbon capturing in the future. For CCU perspective, the bioplastic production that using CO_2 as feedstock via electrochemical and bio-synthesis processes is not carbon negative, but this product has environmental benefits compared to other bioplastic raw materials and fossil-fuel based plastics, such as glucose-based bioplastic and PET. Future work should consider the need for technological advancements to improve efficiency of bioplastic synthesis based on this manufacturing process and reduce the environmental implications, such as using renewable energy resources and sustainable chemicals. In addition, depending on the social perspective, the consumers are willing to adopt and pay more for this sustainable product due to the lower environmental implications. Nevertheless, the cost of new sustainable product is a significant factor that influence the decision. Consequently, the decision-makers should implement regulations to reduce the production cost and encourage companies and industries to produce this sustainable good in a large scale.

6.2. Future work

Future research on CCUS technologies should comprehensively extend environmental impact assessments across the entire lifecycle, integrating detailed analyses of end-of-life management. Technological innovation needs to focus on enhancing material efficiency and reducing the energy demands of CCUS processes, potentially by integrating renewable energy sources such as solar or wind to lower the overall carbon footprint. Furthermore, an estimation of economic viability and policy frameworks is essential to identify supportive financial mechanisms and regulatory environments that facilitate broader adoption.

From the social perspective, further research should focus on the complex interactions between consumer behavior, market forces, and sustainable technologies. Utilizing tools like ABM to simulate various scenarios can provide valuable insights into how social networks, economic incentives, and policy interventions could influence the adoption rates of sustainable CCUS products. Additionally, cross-cultural studies are essential to understand regional differences in consumer behavior and acceptance of sustainable technologies. These studies would help communication strategies and educational programs that effectively address the sociodemographic variations in environmental consciousness and willingness to engage with new technologies.

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Appendix A

Electronic supplemental information from Chapter 2.

Table A1. Life cycle inventories of 1 kg natural wollastonite extraction, comminution, spreading and disposal.

Inventories	**Total amount**	**Unit**	**SimaPro Entries**
Extraction			
Wollastonite blasting	0.000145	kg	Blasting {RoW}| processing | Alloc Def, U
Wollastonite drilling	$3.35 * 10^{-5}$	hr/kg	Loader operation, large, NE-NC/RNA
Loading to truck	$3.35 * 10^{-5}$	hr/kg	Loader operation, large, NE-NC/RNA
Transport to crushing	1	kgkm	Transport, freight, lorry 16-32 metric ton, EURO4 {GLO}| market for | Alloc Def, S
Comminution			
Electricity	0.0055	kWh	Electricity, medium voltage {US}| market group for | Alloc Def, U
Loading to truck	$3.35 * 10^{-5}$	hr/kg	Loader operation, large, NE-NC/RNA
Transport to field	65	kgkm	Transport, freight, lorry 16-32 metric ton, EURO4 {GLO}| market for | Alloc Def, S
Spreading on field			
Loading to truck	$3.35 * 10^{-5}$	hr/kg	Loader operation, large, NE-NC/RNA
Diesel in spreader	0.00173	kg	Diesel, low-sulfur {RoW}| market for | Alloc Def, U
Dissipative flows			
Calcium carbonate	0.86	kg	
Silicon dioxide	0.52	kg	

Table A2. Life cycle inventories of 1 kg wollastonite synthesize, transport and spreading.

Inventories	Total amount	Unit	SimaPro Entries
Raw Materials			
Citric acid	5.53	kg	Citric acid {GLO}| market for | Alloc Def, S
Calcium nitrate	2.35	kg	Calcium nitrate {GLO}| market for | Alloc Rec, S
Ammonium nitrate	2.82	kg	Ammonium nitrate, as N {GLO}| market for | Alloc Def, S
Oxygen	1.38	kg	Oxygen, liquid {RoW}| market for | Alloc Def, S
Silicon dioxide	0.22	kg	Silica sand {GLO}| market for | Alloc Def, S
Synthesis processes			
Electricity	8.48	kWh	Electricity, medium voltage {US}| market group for | Alloc Def, S
Transportation	65	kgkm	Transport, freight, lorry 16-32 metric ton, EURO4 {GLO}| market for | Alloc Def, S
Spreading on field			
Diesel in spreader	0.00173	kg	Diesel, low-sulfur {RoW}| market for | Alloc Def, U
Dissipative flows			
Calcium carbonate	0.86	kg	
Silicon dioxide	0.52	kg	
Air emission			
Carbon dioxide	7.6	kg	

Table A3. Environment and human health impacts comparisons of seven electricity generation resources for natural wollastonite scenario. The most environmentally intensive electricity option for each category is highlighted in green, and the least environmentally.

	OD	GW	SM	AC	EU	HHc	HHnc	RE	ET	FFD
Grid	6.23E-09	3.08E-02	7.46E-03	2.94E-04	7.20E-05	1.06E-09	7.23E-09	3.30E-05	2.07E-01	7.35E-02
Wind	5.74E-09	2.63E-02	7.34E-03	2.78E-04	3.47E-05	7.48E-10	6.10E-09	1.85E-05	1.89E-01	7.00E-02
Biomass	5.72E-09	2.65E-02	9.07E-03	2.83E-04	3.44E-05	7.08E-10	5.99E-09	1.84E-05	1.64E-01	6.99E-02
Coal	5.93E-09	3.33E-02	7.69E-03	2.98E-04	6.71E-05	1.12E-09	7.28E-09	1.97E-05	2.00E-01	7.13E-02
Oil	4.38E-09	9.02E-02	4.00E-03	8.47E-04	3.88E-05	7.83E-10	6.43E-09	2.62E-05	1.79E-01	9.90E-02
PV	5.83E-09	2.67E-02	7.37E-03	2.81E-04	3.76E-05	7.58E-10	6.49E-09	1.92E-05	2.00E-01	7.04E-02
Nuclear	5.73E-09	2.62E-02	7.35E-03	2.79E-04	3.42E-05	6.98E-10	6.00E-09	1.85E-05	1.65E-01	7.00E-02

Table A4. Environment and human health impacts comparisons of seven electricity generation resources for synthetic wollastonite scenario. The most environmentally intensive electricity option for each category is highlighted in green, and the least environmental.

	OD	GW	SM	AC	EU	HHc	HHnc	RE	ET	FFD
Grid	1.29E-05	107.62	5.27	0.549	0.321	4.16E-06	2.111E-05	0.103	752.69	82.47
Wind	1.22E-05	100.48	5.10	0.523	0.263	3.67E-06	1.935E-05	0.081	725.11	77.08
Biomass	1.21E-05	100.85	7.78	0.532	0.263	3.61E-06	1.918E-05	0.080	685.99	76.97
	05					4.25E-06	2.120E-05	0.082	741.81	79.02
Oil	1.72E-05	121.85	6.85	0.695	0.277	3.73E-06	1.987E-05	0.092	710.06	122.09
Coal	1.24E-	111.41	5.64	0.555						0.313

PV	1.22E-05	101.15	5.13	0.527	0.267	3.69E-06	1.997E-05	0.081	742.95	77.65
Nuclear	1.22E-06	100.47	5.11	0.526	0.262	3.59E-06	1.919E-05	0.081	686.48	77.03

Table A5. Impacts comparison of two scenarios considered in this study according to surface area (1 m^2/g) as functional unit.

Impact categories	**Unit**	**Synthesis scenario**			**Natural scenario**
		60%	80%	99%	
Environmental impacts					
Ozone depletion (OD)	kg CFC-11 eq	2.40×10^{-7}	1.80×10^{-7}	1.46×10^{-7}	2.33×10^{-10}
Global warming (GW)	kg CO_2 eq	2.14	1.60	1.29	1.15×10^{-3}
Smog (SM)	kg O_3 eq	9.85×10^{-2}	7.39×10^{-2}	5.97×10^{-2}	2.79×10^{-4}
Acidification (AC)	kg SO_2 eq	1.02×10^{-2}	7.69×10^{-3}	6.21×10^{-3}	1.10×10^{-5}
Eutrophication (EU)	kg N eq	5.99×10^{-3}	4.49×10^{-3}	3.63×10^{-3}	2.70×10^{-6}
Ecotoxicity (ET)	CTUe	14.10	10.50	8.52	7.74×10^{-3}
Fossil fuel depletion (FFD)	MJ surplus	1.54	1.16	0.93	2.75×10^{-3}
Human health impacts					
Carcinogenic (HHc)	CTUh	7.78×10^{-8}	5.83×10^{-8}	4.71×10^{-8}	3.99×10^{-11}
Non-carcinogenic (HHnc)	CTUh	3.94×10^{-7}	2.96×10^{-7}	2.39×10^{-7}	2.71×10^{-10}
Respiratory effects (RE)	kg PM2.5 eq	1.93×10^{-3}	1.44×10^{-3}	1.17×10^{-3}	1.24×10^{-6}

Grid Wind Biomass

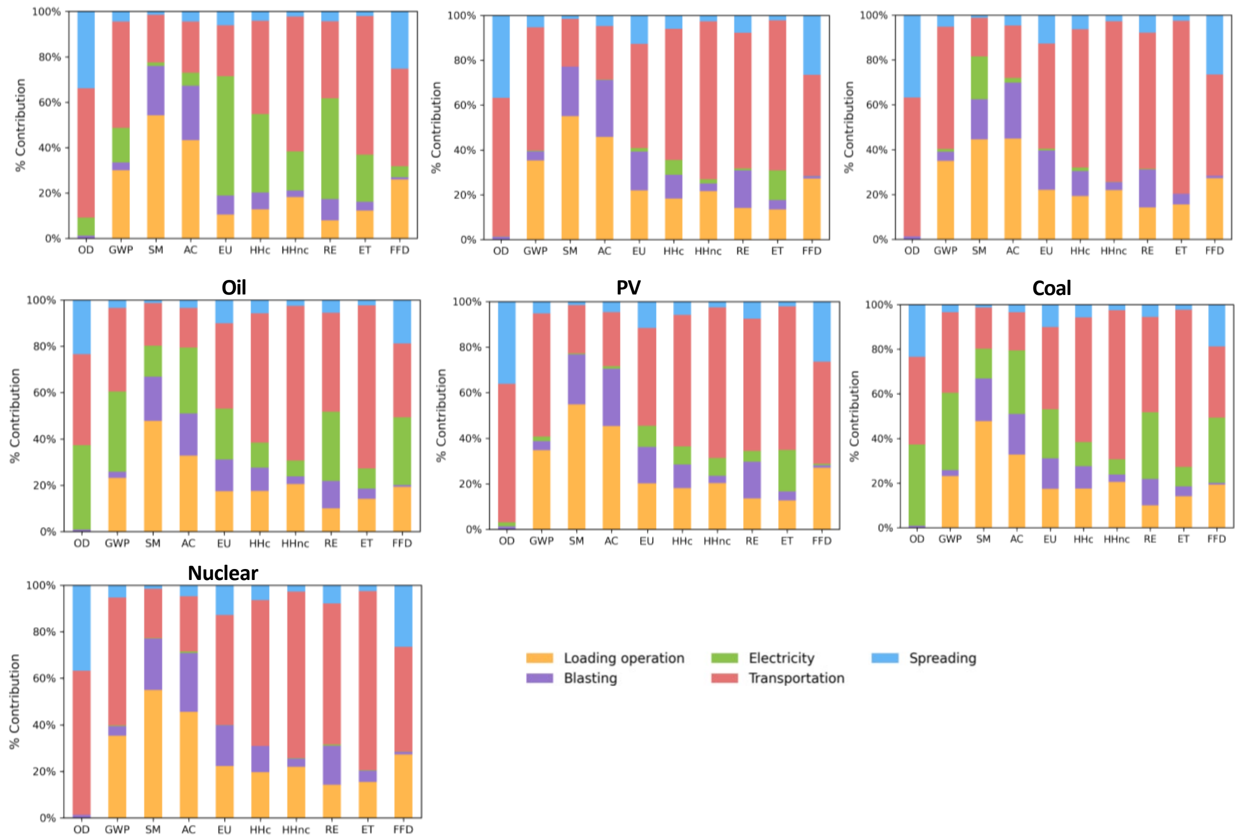

Figure A24. The contribution of processes to all impacts of natural wollastonite scenario based on different electricity resources.

Grid **Wind** **Biomass**

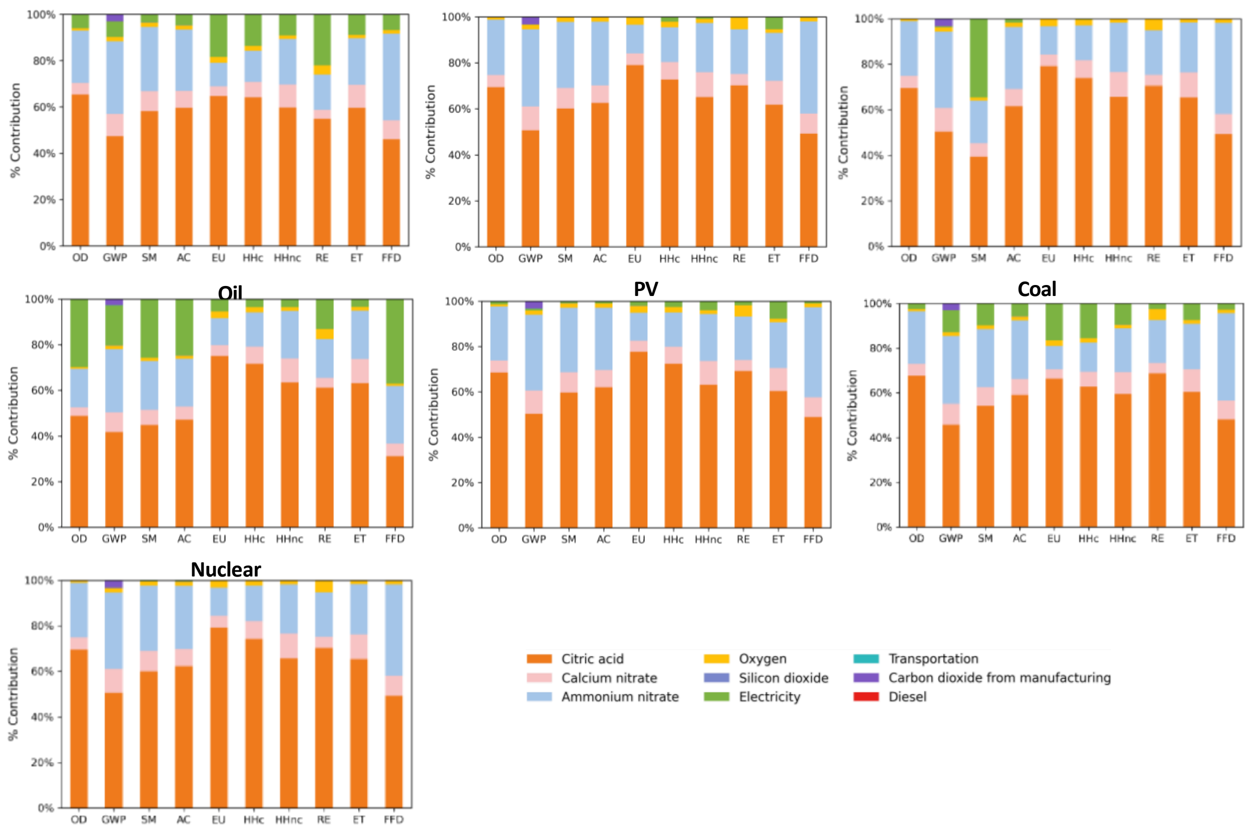

Figure A25. The contribution of reagents and processes to all impacts of synthetic wollastonite scenario based on different electricity resources.

Appendix B

Electronic supplemental information from Chapter 3.

Please note that all inventory items used in the analysis are from the Ecoinvent database, version 3.9.1.

Table B1. Inventories of1 gram bioplastic synthesis in the electrochemical process (2686 ppm acetate produced).

Inventories	Total amount	Unit	SimaPro Entries
Carbon monoxide (CO)	19.88	kg	Carbon monoxide {RoW}| market for | APOS, U
DI water	4.42	kg	Water, deionised {RoW}| market for water, deionised | APOS, U
Carbon fiber	0.043	g	Acrylonitrile {GLO}| market for | APOS, U
Copper (Cu)	0.0018	g	Copper-rich materials {GLO}| market for copperrich materials | APOS, U

Silver (Ag)	0.0015	g	Silver {GLO}| market for | APOS, U
Amberchrom® 50WX8	5.52	g	Polystyrene, general purpose {GLO}| market for | APOS, U
Electricity	0.66	kWh	Electricity, low voltage {US}| market group for | APOS, U

Table B2. Inventories of 1 gram bioplastic produced in the bio-synthesis process.

Inventories	**Total amount**	**Unit**	**SimaPro Entries**
Ammonium sulfate	0.038	g	Ammonium sulfate {RoW}| market for ammonium sulfate | APOS, U
Magnesium sulfate	0.018	g	Magnesium sulfate {GLO}| market for | APOS, U
Sodium bicarbonate	0.45	g	Sodium bicarbonate {GLO}| market for sodium bicarbonate | APOS, U
Monosodium phosphate	1.53	g	Sodium phosphate {RER}| production | APOS, U
Nickel sulfate	0.00013	g	Nickel sulfate {GLO}| market for | APOS, U
Monopotassium phosphate			
Potassium hydroxide	0.078	g	Potassium hydroxide {RoW}| production | APOS, U
Phosphoric acid	0.11	g	Phosphoric acid, fertiliser grade, without water, in 70% solution state {US}| phosphoric acid production, dihydrate process | APOS, U
Ferric citrate			
Iron(III) chloride	0.007088	g	Iron (III) chloride, without water, in 40% solution state {GLO}| market for | APOS, U
Citric acid	0.00839	g	Citric acid {GLO}| market for | APOS, U
Sodium hydroxide	0.00178	g	Sodium hydroxide, without water, in 50% solution state {RER}| chlor-alkali electrolysis, membrane cell | APOS, U

Table B3. Environmental and human health implications of two processes including CO gas manufacturing for 1 FU produced.

Impact categories	Unit	Electrochemical process	Bio-synthesis process	Total Impact
Environmental impacts				
Ozone depletion (OD)	kg CFC-11 eq	7.08E-05	2.47E-09	7.08E-05
Global warming (GW)	kg CO_2 eq	1.65E-03	2.14E-07	1.65E-03
Smog (SM)	kg O_3 eq	1.83E-03	2.00E-07	1.83E-03
Acidification (AC)	kg SO_2 eq	2.24E-03	5.82E-07	2.24E-03
Eutrophication (EU)	kg N eq	6.63E-03	1.86E-06	6.63E-03
Ecotoxicity (ET)	CTUe	4.45E-03	4.39E-06	4.46E-03
Fossil fuel depletion (FFD)	MJ surplus	6.15E-03	2.32E-07	6.15E-03
Human health impacts				
Carcinogenic (HHc)	CTUh	2.68E-05	2.68E-05	2.68E-05
Non-carcinogenic (HHnc)	CTUh	8.44E-05	8.62E-08	8.45E-05
Respiratory effects (RE)	kg PM2.5 eq	2.44E-07	2.44E-07	2.46E-03

Table B4. Environmental and human health implications of two processes without CO gas production for 1 FU produced.

Impact categories	Unit	Electrochemical process	Bio-synthesis process	Total Impacts
Environmental impacts				
Ozone depletion (OD)	kg CFC-11 eq	1.53E-07	2.47E-09	1.55E-07

Global warming (GW)	kg CO_2 eq	1.48E-05	2.14E-07	1.50E-05
Smog (SM)	kg O_3 eq	7.85E-06	2.00E-07	8.05E-06
Acidification (AC)	kg SO_2 eq	1.16E-05	5.82E-07	1.21E-05
Eutrophication (EU)	kg N eq	9.52E-05	1.86E-06	9.71E-05
Ecotoxicity (ET)	CTUe	2.88E-05	4.39E-06	3.31E-05
Fossil fuel depletion (FFD)	MJ surplus	2.26E-05	2.32E-07	2.29E-05
Human health impacts				
Carcinogenic (HHc)	CTUh	3.96E-07	6.74E-09	4.02E-07
Non-carcinogenic (HHnc)	CTUh	5.36E-07	8.62E-08	6.23E-07
Respiratory effects (RE)	kg PM2.5 eq	2.94E-05	2.44E-07	2.97E-05

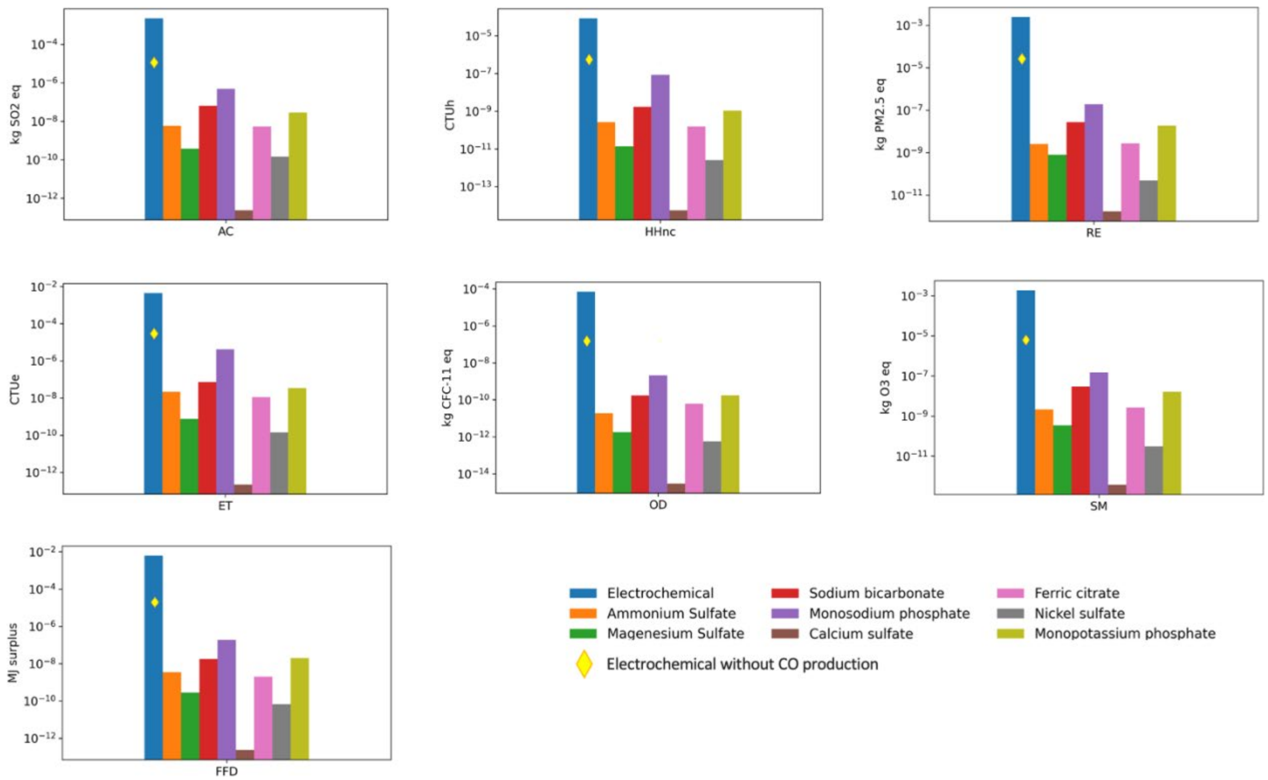

Figure B1. The life cycle distribution of two processes for the rest seven impacts is based on the log scale.

Appendix C

Electronic supplemental information from Chapter 4.

Table C1. Demographic information of respondents and 2020 U.S. census.

Coefficient	% of this survey	% of 2020 U.S. census
Age		
18-24	52.21	9.4
25-34	33.63	13.5
35-44	12.39	12.7
45-64	1.77	25.4
>64	0	16.81
Gender		
Male	29.20	49.1
Female	60.18	50.9
Non-binary	6.19	/
Prefer not to say	3.54	/
Other	0.88	/
Race/ethnicity identification		
Hispanic, Latino, or of Spanish origin	9.73	18.70
White	48.67	50.08
Asian	37.17	4.88
Black or African American	0.88	10.08
Native American or Alaska American	0.88	1.06
Other	2.94	15.12
Education level		

Less than high school or GED	0	9.77
High school graduate or GED	7.96	27.84
College or Associate degree	6.19	10.10
Bachelor's degree (or equivalent)	17.70	22.13
Graduate or Professional degree	34.51	12.66
Some college, no degree	33.63	17.50
Annual income		
<$15,000	20.35	8.35
$15,000-$24,999	3.54	7.44
$25,000-$34,999	6.19	7.62
$35,000-$44,999	11.50	7.18
$50,000-$74,999	8.85	16.23
$75,000-$99,999	13.27	12.33
$100,000-$149,999	7.96	16.42
$150,000-$199,999	5.31	9.15
>$200,000	6.19	11.92
Prefer not to disclose	16.81	/

Results of XGBoost and Logistic regression analysis

The accuracy of this model is 92%. The overall impact of certain features on "willing to pay more" is indicated by its SHAP values over all selected instances, as shown in Figure S1. The main objective of this study is identifying the most impactful features and understanding their patterns of influences, the top nine features will be focused. The negative value means the respondents who have these features are unwilling to pay more to purchase single use bioplastic bottles, especially the managers, the people are strongly agree to decide to buy bioplastic bottles, the respondents who have some college degree and graduate degree, and age between 25 to 34. The positive values represent the increased probability that people are willing to pay more to buy single use bioplastic bottles, especially males, in the age range between 35 to 44, someone who prefers not to tell income, and heard about bioplastic bottles but not able to explain it well.

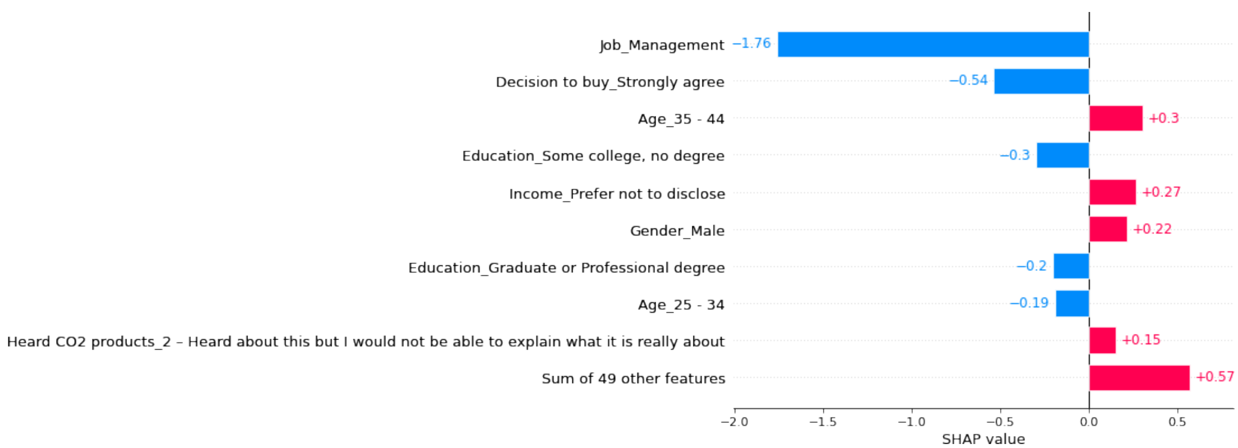

Figure S1. Pay more.

The impact of features on “willing to pay less” is shown in Figure S2. As match the results above, the male, in the age range between 35 to 44, who have heard of bioplastic bottles but cannot explain what it is is willing to pay more, so the SHAP value is negative on “willing to pay less”. In addition, the respondents who have a graduate or professional degree is unwilling to pay less as well. The participants, who work in education instruction and library field and in somewhat agreeing to decide to purchase, decreased the probability of paying less for single use bioplastic bottles. The respondents have the neutral fashion of environmental consciousness, bring their own water bottles every day, and rarely to bring water bottles are willing to pay less for single use bioplastic bottles.

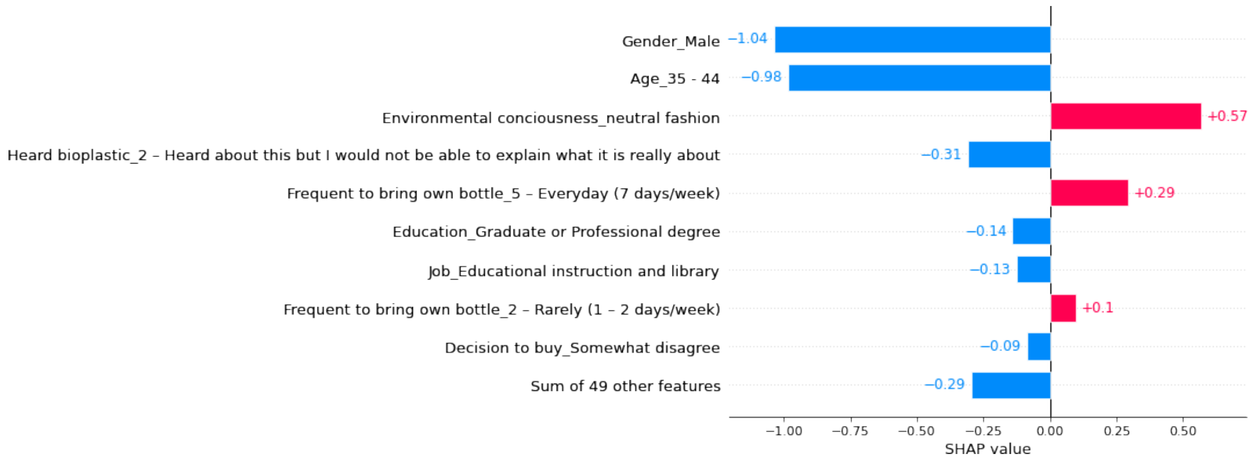

Figure S2. Pay less.

For the same amount of payment of single use bioplastic bottles compared to conventional plastic bottles (Figure S3), the respondents who are male, have management occupation, have graduate or professional degrees, heard of bioplastic bottles and can describe the brief definition, and in the age range between 25 to 34 are willing to pay the same price to buy the single use bioplastic bottles. The participants who do not prefer to tell their income are unwilling to pay the same amount because they are willing to pay more to purchase this kind of product. Additionally, the people who bring their own water bottles every day decreased the probability of paying the same price to buy this product, because they have reusable water bottles and do not need the single use water bottles anymore. The group that heard about bioplastic bottles but was unable to explain it was unwilling to pay the same price because they were willing to pay more to purchase bioplastic bottles, which matched the results above.

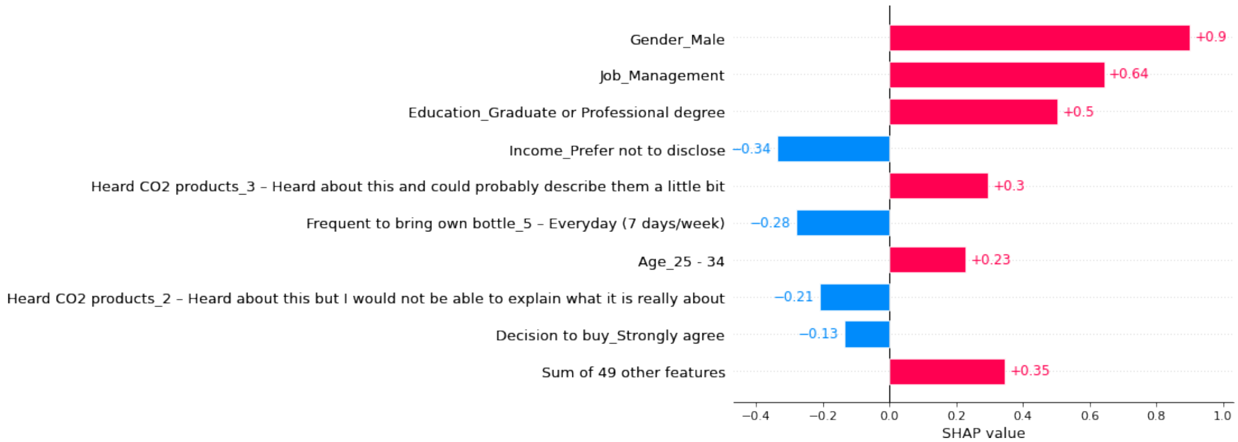

Figure S3. Pay same

Few respondents are unwilling to pay for single use bioplastic bottles (Figure S4), who strongly agree to buy bioplastic bottles, having some college no degree, and in age range between 25 to 34. However, the participants, who have neutral fashion or extremely passionate environmental consciousness, income range in $25,000 to $34,999, are familiar with bioplastic bottles and able to explain well, bring their own water bottles every day or very often, are willing to buy bioplastic bottles.

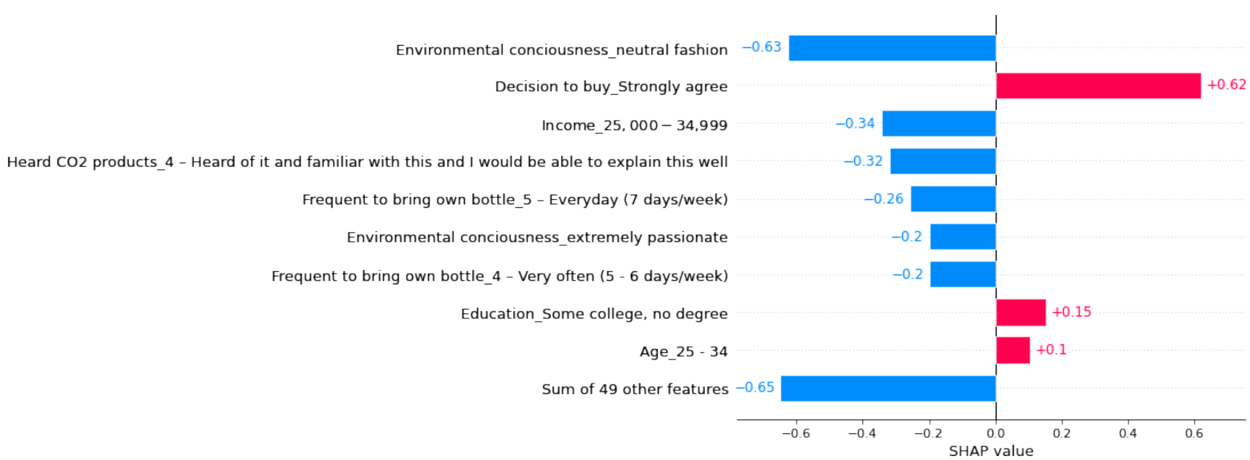

Figure S4. Not willing to pay.

<u>Details of Survey 1</u>

1. Introduction

In this survey, we seek to understand the willingness to pay for CO_2 captured bioplastic bottles. The survey will gain valuable insights into the bioplastic bottles replace conventional plastic bottles. This is related to environmental awareness, perceived knowledge about carbon captured and utilization (CCU) products, CCU product purchase preference, and the socioeconomic for customers.

2. Consent Form

You are invited to participate in a research study about the willingness to pay for CO_2 captured bioplastic bottles. You have been asked to participate because you are identified as a plastic bottle customer. The purpose of the research is to understand the bioplastic bottle purchase behavior and the awareness of climate change.

If you decide to participate in this research, you will be asked to do a survey, which includes a series of questions regarding your willingness to pay for carbon captured and utilization products (i.e. bioplastic bottle). There are 4 parts involved in this survey. Your participation will last approximately 15 min in total.

There are no risks associated with participating in this study. The study is anonymous. Neither your name nor any other identifiable information will be recorded. Neither your name nor any other identifiable information will be published. Only authorized researchers will have access to the data and the protection and security measures of the data.

193

3. Questionnaire

Part 1: Climate change awareness

1. Have you heard about concerns related to increased carbon dioxide emissions and global warming?

   a) Yes
   b) No

   c) Unsure

2. Do you believe that increased carbon dioxide emissions are a problem? a) Yes

   b) No

   c) Unsure

3. If you said "Yes, I believe that increased carbon dioxide emissions are a problem" in question 2, which reason seems most significant and relevant to you?

   a) Human health effects

   b) Economic effects

   c) Environmental impacts

   d) Other (text entry box)

4. If you said "No, I don't believe that increased carbon dioxide emissions are a problem in question 2", indicate the reason that the carbon dioxide emissions issue seems irrelevant to you.

   a) I can't feel it in my daily life

b) I can't change anything

c) Insufficient information

d) I'm not interested in this topic

e) Other (text entry box)

5. Are you currently trying to reduce your personal carbon dioxide emissions? a) Yes, I am

b) No, I am not

c) I don't know

<u>Part 2: Perceived knowledge about carbon capture and utilization (CCU) products</u>

1. Have you heard about products where carbon dioxide is removed from the air and used as a carbon source for products before today? (text entry box)

1 – Never heard of it

2 – Heard about this but I would not be able to explain what it is really about

3 – Heard about this and could probably describe them a little bit

4 – Heard of it and familiar with this and I would be able to explain this well

5 – I'm very familiar with this and I can tell everything

2. When I think of capturing carbon dioxide and using it as a raw material to make products for use by people, it makes me feel:

a) Enthusiastic

b) Delight

c) Pride

d) Afraid

e) Interested

f) Worried

g) Nervousness

h) Risky

i) Disgust

j) Disinterested

3. I have heard about captured carbon being used in: (text entry box)

Part 3: CCU Product Purchase Behavior

One product that is being considered for being made with captured carbon is the bioplastic bottle. Bioplastic bottles are used to substitute conventional plastic bottles in the future due to the lower fossil fuel resource usage, smaller carbon footprint, and faster decomposition.

1. How often do you bring your own water bottle when you go to school/work or hang out?

   (text entry box)

   1 – Never (0 day/week)

   2 – Rarely (1 – 2 days/week)

   3 – Sometimes (3 - 4 days/week)

   4 – Very often (5 - 6 days/week)
   5 – Everyday (7 days/week)

2. What is the major type of reusable water bottle you currently used?

    a) Plastic

    b) Aluminum

    c) Stainless steel

    d) Glass

    e) Other (text entry)

3. How many single use plastic bottles do you use on average per week: (text entry box)

4. Have you heard of bioplastic bottles in general? (text entry box)

    1 – Never heard of it

    2 – Heard about this but I would not be able to explain what it is really about

    3 – Heard about this and could probably describe them a little bit

    4 – Heard of it and familiar with this and I would be able to explain this well

    5 – I'm very familiar with this and I can tell everything

5. Which type of bioplastic have you heard of before?

    a) Starch-based bioplastic

    b) Cellulose-based bioplastic

    c) Protein-based bioplastic

    d) Aliphatic polyesters
    e) Organic polyethylene

    f) Just bioplastics generally

g) Other (text entry)

h) None of them

6. If you have not bought or used bioplastic bottles yet, what keeps you from buying or using them?

   a) Health/safety concerns

   b) Lack of information about the products

   c) Limited awareness

   d) Limited availability

   e) Design

   f) Low quality

   g) High cost

   h) Others: (text entry box)

7. The environmental impact of the bioplastic bottle factor into your decision to buy this product?

   1 – Strongly disagree

   2 – Disagree

   3 – Neutral

   4 – Agree

   5 – Strongly agree

8. What price point you would buy the bioplastic bottles when compared to the conventional single use plastic bottle?

a) 200% more

b) 100% more

c) 75% more

d) 25% more

e) Same amount

f) 25% less

g) 75% less

h) 100% less (free)

9. Which of the factors shown below are important for you when selecting biobased plastic bottles? (select all that apply)

a) Price

b) Durability

c) Compostability

d) Biodegradability

e) Recyclability

f) Reusability

g) Raw materials

h) Aesthetics

i) Environmental footprint
j) Others: (text entry box)

10. Ranking these factors from 1 (least important) to 10 (most important)

- Price

- Durability
- Compostability
- Biodegradability
- Recyclability
- Reusability
- Raw materials
- Aesthetics
- Environmental footprint
- Others: (text entry box)

Part 4: Socio-demographic information

1. Which age group can describe you?

    a) < 18

    b) 18 – 25

    c) 26 – 35

    d) 36 – 45

    e) 46 – 55

    f) 56 – 65

    g) > 66
2. Which gender do you most closely identify with?

    a) Female (includes both cis and transgendered)

    b) Male (includes both cis and transgendered)

    c) Nonbinary

    d) Other: (text entry box)

    e) Prefer not to answer

3. What race/ethnicity identifies you most closely?

a) White, not Hispanic

b) Black

c) Native American, Eskimo, Aleut

d) Asian and Pacific Islander

e) Hispanic Origin (of any race)

f) Two or more races

g) Prefer not to answer

4. What is the highest education level you have completed?

a) Less than high school diploma or GED

b) High school diploma or GED

c) College or Associates degree

d) Bachelor's degree (or equivalent)

e) Graduate or Professional degree

5. Which of the following best described your occupation?

a) Management

b) Office and administrative support

c) Sales and related

d) Educational instruction and library

e) Healthcare practitioners and technical

f) Production

g) Food preparation and serving related

h) Business and financial operations

i) Construction and extraction

j) Computer and mathematical

k) Transportation

l) Building and grounds cleaning and maintenance

m) Material moving

n) Healthcare support

o) Installation, maintenance, and repair

p) Personal care and service

q) Arts, design, entertainment, sports, and media

r) Architecture and engineering

s) Protective service

t) Community and social service

u) Legal
v) Life, physical, and social science

w) Farming, fishing, and forestry

6. What is your total household annual income?

a) ≤ $15,000

b) $15,000 - $24,999

c) $25,000 - $34,999

d) $35,000 - $44,999

e) $50,000 - $74,999

f) $75,000 - $99,999

g) \$100,000 - \$149,999

h) \$150,000 - \$199,999

i) ≥ \$200,000

7. Which of the following best described your environmental consciousness?

a) In reality, I don't particularly care about the environment

b) For me, there are more important things than environmental issues

c) Companies and industries should take more efforts than individuals to improve the environment because an individual inaction will not significantly influence the environment

d) Honestly, I don't know what behaviors are good or bad for the environment

e) I don't know how much media information on the environment is reliable

f) Environmental issues are significant problems to be solved

g) I have switched products for environmental reasons

h) I purchase the less harmful products to other people and the environment when I have choice

i) I'm really enthusiastic and have passion to improve the environment

Details of Survey 2

Bioplastic Water Bottle Survey

This survey is a part of a UW-Madison research project, in which participation involves taking a brief anonymous survey. Participation is voluntary and any questions about the research can be asked of the researcher who is administering the survey. By checking the box below, you confirm you are (18+) and provide consent to participate in the research.

☐ Yes!

1. If a typical plastic bottle of water (20 ounces) costs $2.00 at the local store, how much total would you be willing to pay for a bottle of water where the plastic was made from carbon dioxide (CO2) taken out of the air? (select the highest amount you would be willing to pay)

    a. $0.00 (it would need to be free)
    b. $0.50
    c. $0.75
    d. $1.00
    e. $1.25
    f. $1.50
    g. $1.75
    h. $2.00 (Same price)
    i. $2.25
    j. $2.50

k. $3.00 1. $3.25

m. $3.50

n. $3.75

o. $4.00

p. $5.00

q. $6.00

r. I would not purchase any plastic bottle of water, regardless of the price

2. Do you believe climate change is real and occurring?

a. Yes

b. No

c. Unsure

3. Do you believe that climate change is due to the actions of people? a. Yes

b. No

c. Unsure

4. Which option best describes your attitude towards the environment?(select all that apply)
a. In reality, I don't particularly care about the environment

b. For me, there are more important things than environmental issues

c. Companies and industries should take more efforts than individuals to improve the.

environment because an individual inaction will not significantly influence the environment

d. Honestly, I don't know what behaviors are good or bad for the environment

e. I don't know how much media information on the environment is reliable

f. Environmental issues are significant problems to be solved

g. I have switched products for environmental reasons

h. I purchase the less harmful products to people and the environment when I have a choice

i. I'm really enthusiastic and have passion to improve the environment

Appendix D

Electronic supplemental information from Chapter 4.

Table D1. The average value, differences, and standard deviation of zero, four, and eight neighbors.

	Average cumulative # of bioplastic water bottle adoption	Average cumulative # of conventional water bottle adoption	Differences (compared to 0 neighbor)	Differences (compare to 4 neighbors)	Standard deviation (compare to 0 neighbors)	Standard deviation (compare to 4 neighbors)
No neighbor	100845.15	61654.85				
4 neighbors	100825.04	61674.96	-20.11		14.22	
8 neighbors	100770.56	61729.44	-74.59	-54.47	52.74	38.52

Table D8. The average cumulative value of bioplastic water bottle adoption is based on the influence of neighbors.

The weighting of neighbors' change (W10)	Average cumulative # of bioplastic water bottle adoption (8 neighbors)	Standard deviation	95% confidence interval
0 (no neighbor)	100517.5	1.61	(384.81, 385.44)
0.1	100590.3	1.77	(385.05, 385.76)
0.2	100674.13	1.69	(385.39, 386.06)
0.3	100739.3	1.66	(385.65, 386.30)
0.4	100754.23	1.50	(385.73, 386.33)
0.5 (baseline)	100798.71	1.29	(385.95, 386.46)
0.6	100839.59	1.20	(386.12, 386.60)
0.7	100860.03	1.32	(386.18, 386.70)
0.8	100911.63	1.11	(386.41, 386.85)
0.9	100939.73	1.12	(386.52, 386.96)
1	100976.96	0.91	(386.71, 387.06)

Survey data used in this study

11. What price point you would buy the bioplastic bottles when compared to the conventional single use plastic bottle?

    i) 200% more

    j) 100% more

    k) 75% more

    l) 25% more

    m) Same amount

    n) 25% less

o) 75% less

p) 100% less (free)

12. Which of the factors shown below are important for you when selecting biobased plastic bottles? (select all that apply)

k) Price

l) Durability

m) Compostability

n) Biodegradability

o) Recyclability

p) Reusability

q) Raw materials
r) Aesthetics

s) Environmental footprint

t) Others: (text entry box)

13. Ranking these factors from 1 (least important) to 10 (most important)

- Price
- Durability
- Compostability
- Biodegradability
- Recyclability
- Reusability
- Raw materials
- Aesthetics
- Environmental footprint
- Others: (text entry box)

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