Computers and Chemical Engineering 179 (2023) 108455

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/cace

Simulation tools for net-positive process design: Trees as unit operations for carbon sequestration and air quality regulation

Yazeed M. Aleissa [a,b], Bhavik R. Bakshi [b,c,d,e,*]

[a] Department of Chemical and Materials Engineering, Faculty of Engineering, King Abdulaziz University, Jeddah, Saudi Arabia
[b] William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH 43210, United States
[c] School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ, 85287, United States
[d] School of Sustainability, Arizona State University, Tempe, AZ, 85287, United States
[e] School of Complex Adaptive Systems, Arizona State University, Tempe, AZ, 85287, United States

ARTICLE INFO

Dataset link: https://doi.org/10.5281/zenodo.7387087

Keywords:
Ecosystem services
Process design
Simulation
Sustainable engineering
Carbon sequestration
Air pollution

ABSTRACT

Chemical processes have significant environmental and societal impacts, such as climate change and human health, due to air and water pollution. In addition, chemical processes consume unsustainable amounts of natural ecosystems' goods and services. Engineers have tried to address these challenges by reducing waste, integrating processes, and minimizing the consumption of raw materials and energy. However, these efforts have not been enough to address the impact of the process on natural ecosystems and local communities. Hence, the need to integrate ecological systems into traditional engineering design to provide sustainable and cost-effective solutions. Although models for ecological systems are readily available in the literature, engineers are hesitant to utilize these models without familiar tools and the traditional undervaluation of ecosystem services' role and the uncertainty of their performance. To overcome some of these barriers, ecosystems can be classified as unit operations since they can be designed to achieve specific tasks. This work focuses on integrating vegetation as unit operations in process design to remove air pollutants and sequester carbon. We developed a practitioner-friendly simulation module in CHEMCAD that utilizes sophisticated rural and urban forestry models developed by the online i-Tree assessment tool. We demonstrate the module through a power plant case study and highlight some alternative spatially explicit integrated designs that are environmentally and economically superior.

1. Introduction

Numerous countries and various corporations have been seeking solutions that not only reduce their environmental and societal impacts of global warming and air pollution but also go beyond these conventional goals to ensure that their net impact on ecosystems and society is positive. To encourage nature-positive and people-positive decisions (Obura et al., 2023), the United Nations (UN) has declared 2021–2030 as the UN decade on ecosystem restoration (UNEP, 2022). In recent years, many countries, cities, and organizations have shown interest in nature-based solutions, which include sustainable designs that promote the adaptation and resilience of natural features in engineering practice and management (Cohen-Shacham et al., 2016). One of the top adopted solutions is planting trees and restoring local ecosystems to mitigate the environmental impact of global warming and air pollution and improve human well-being. The many ecological and societal benefits of trees are well documented (Nowak et al., 2014) using sophisticated models (I-Tree, 2016) based on scientific understanding (Smith, 1990). Although nature-based solutions require knowledge from ecology, engineering, and social sciences, the concept of ecosystem goods and services (Millennium Ecosystem Assessment, 2005) and monetary valuation (Costanza et al., 1997) have encouraged research and collaboration between different disciplines. However, the systematic adoption of nature-based solutions in engineering and process design has been mainly limited to academic research, and Dow Chemical is an exception. They have worked on the role of trees and wetlands and even developed the Ecosystem Services Identification & Inventory (ESII) tool (Rogers et al., 2023).

Historically, the environment was not a part of process design. Instead, companies were forced to comply with environmental regulations from government agencies. However, this approach resulted in economic loss for companies and was not enough to limit the ecological damage. This led to adopting new design approaches to produce less waste (Friedlander, 1989) and to use recycling for chemicals and other

* Corresponding author.
E-mail address: bhavik.bakshi@asu.edu (B.R. Bakshi).

https://doi.org/10.1016/j.compchemeng.2023.108455
Received 4 August 2023; Received in revised form 6 October 2023; Accepted 7 October 2023
Available online 10 October 2023

Nomenclature

Acronyms

EAC	Equivalent annualized cost
ES	Ecosystem goods and services
FGD	Flue gas desulfurizer
PM	Particulate matter
SCR	Selective Catalytic Reducer

Indices

i	US counties
j	Pollutant species ∈ {CO_2, CO, NO_2, O_3, SO_2, PM}

Parameters

α	Canopy cover percentage
α^{design}	Design canopy cover percentage
β	Epidemiology effect coefficient
A_v	Vegetation covered area
A_{water}	Water covered area
$A_{developed}$	Developed area
A^{design}	Minimum design area
C	Pollutant concentration
F	Vegetation uptake
f^{uptake}	Vegetation uptake factor
f^{health}	Health impact factor
m^{total}	Annual pollutant mass removal
$m^{Process}$	Process annual emission
n	Project life span
P	Population size
r	Discount rate
v^d	Deposition velocity
V^{total}	Annual value of pollutant removal
Y_0	Baseline incidence rate
ΔY	Change in the number of health effects

valuable resources (El-Halwagi, 1997; Mizsey, 1994). One of the first methods of process design with environmental consideration was the waste reduction algorithm (WAR) (Cabezas et al., 1999), which objective was to minimize the waste production while having acceptable economics. More advanced design methods have been developed to integrate processes through utilizing material and energy flows to use less energy and raw materials, and subsequently at lower costs (Chertow, 2000). Such examples include the optimization of resources used to design heat exchanger networks (Pan et al., 2013), material use and by-products (Cimren et al., 2011), and design of equipment and unit operations (Pan et al., 2016). Other approaches focused on assessing the environmental impact of processes, such as Life Cycle Assessment (LCA), which quantified the impact of the design process and the impact that the process caused. The implementation of LCA in process design has been widely used to reduce the impact of the process in terms of total emissions (Eliceche et al., 2007).

However, all previous approaches focused on the indirect implementation of nature in process design, such as how it is being impacted through pollution, emissions, and resource extraction. Or through evaluating the magnitude of the environmental impact in the case of LCA. One of the first approaches to directly account for the capacity of natural system and include it in process design was the concept of techno-ecological-synergy (TES) (Bakshi et al., 2015), which assess the sustainability and performance of process systems and explores their synergies with local ecological systems. However, putting ecological solutions on par with traditional technological solutions requires informative comparisons between efficiency, reliability, impact, and cost to help decision makers select practical designs for sustainable systems. Hence, Gopalakrishnan and Bakshi (2018) proposed including ecosystem services as unit operations in process design. Although ecosystems simultaneously provide multiple services, they can be designed to perform a specific task similar to technological equipment (McCabe and Smith, 1957). Thus, the TES concept demonstrated promising results when natural systems were incorporated into the design and decision-making processes. Examples such as including trees to mitigate air pollution (Gopalakrishnan et al., 2016) and constructed wetlands for water quality regulation (Aleissa and Bakshi, 2021a) in industrial designs have demonstrated superior designs with considerable environmental and economic benefits.

However, adopting nature-based solutions in engineering designs presents numerous challenges. First, most engineers are unfamiliar with ecological models and the various factors that can affect the design's performance and cost. Engineers usually require accessible models and information regarding systems to compare the different alternative designs. In addition, engineers considerably underestimate the value of the goods and services provided by natural systems and the benefits they provide to industry and local communities.

This study addresses these challenges and facilitates the adoption of nature-based solutions in chemical process design through the following novel contributions. We highlight the integration of the vegetation ecosystem in process design and focus on carbon sequestration and air quality regulation services. We compare the performance of the vegetation ecosystem services with the performance of current technological alternatives that perform the same tasks. Further, we develop a vegetation simulation module for the CHEMCAD simulation software and demonstrate this module in the context of a power plant case study. We compare the vegetation performance for limiting CO_2 and air pollutants emissions with other control equipment. We find that integrated designs provide attractive solutions to reduce the total cost and environmental and social impacts of the process. The developed module can be used to determine the location of the process by examining the spatial variation of the vegetation ecosystem, which can be tailored to specific designs. We also emphasized the importance of the benefits of ecosystem services and their role in achieving goals such as net-zero emissions and nature- and people-positive decisions. We show how our software tool can guide progress toward goals such as net-zero pollution and net-zero health impact cost. To enable other engineering researchers, we make our CHEMCAD model available for further development (Aleissa and Bakshi, 2023), thereby adding to the CHEMCAD implementation of treatment wetlands, which was made available in our previous work (Aleissa and Bakshi, 2021a,b).

2. Background

2.1. Vegetation ecosystem services

In general, the vegetation ecosystem and trees, in particular, provide multiple goods and services to humans. This includes the supply of timber, firewood, and food. In addition, they provide services such as temperature regulation, sequestration and storage of carbon, and air quality regulation. They play a crucial role in water and nutrient cycling, maintenance of soil quality, erosion prevention, and water filtration. Moreover, they are essential for sustaining biodiversity by providing habitat to animals, insects, birds, and other living organisms. Lastly, they provide space for recreational activities and have aesthetic, cultural, and spiritual values that directly contribute to human well-being (Bakshi, 2023; Tyrväinen et al., 2005; Riis et al., 2020). However, vegetation ecosystems can also provide disservices if they are not properly managed, such as the increased pollution levels due to reduced air exchange from wind blocking (Delshammar et al., 2015; Escobedo et al., 2011). In addition, trees can produce pollen and precursors of air pollutants such as biogenic volatile organic compounds, which have direct health effects and impact air quality (Lyytimäki et al., 2008; Von Döhren and Haase, 2015).

2.2. Reforestation for climate change mitigation

There has been a growing interest in using trees to reduce the severity of the effects of climate change. Trees offer attractive and inexpensive solutions at different scales, from small communities to countries and global initiatives (World Economic Forum, 2020). However, there are numerous factors to consider for reforestation projects, including species, location, land conditions, and other ecosystems, which considerably affect the success of the project. For example, many researchers and experts advocate planting trees on former forest land and avoiding the conversion of other ecosystems, such as wetlands, into new forests (FAO and SER, 2021). This is necessary to prevent the destruction of other ecosystems. Further, planting various native species will help trees grow and flourish naturally, providing additional benefits.

Approaches for planting trees are implemented as a part of forest ecosystem restoration and rehabilitation or as tree plantation. Plantations are uniform agroecosystems that lack the unique characteristics and biodiversity of native forest ecosystems. Plantations are promoted as carbon sink projects and usually implemented as monoculture or near-monoculture systems. Monoculture plantation refers to the reforestation of land with a single species to maximize benefits at a low cost. However, different studies show that this approach may produce fewer benefits than native ecosystems (Liu et al., 2018). In addition, plantations are likely to be less resilient than restoration and require more human intervention. Further, adverse effects on local ecosystems can be observed after a large-scale plantation project is implemented. These include changes in the hydrological cycle, reduction in water quantity and quality, loss of wildlife and useful plants, and soil erosion (World Rainforest Movement, 1999). Another adverse impact of monoculture plantations is the increased potential risk of wildfires. Extreme conditions such as dry weather and dry spell periods can assist plantation wildfires (Hermoso et al., 2021; Gómez-González et al., 2018). Moreover, if the burned area were not properly managed and rehabilitated for natural restoration and regrowth, there would be a high chance for another wildfire (Thompson et al., 2007). Conversely, the strategy to restore ecosystems aims to increase forest goods and services rather than maximize tree cover, in addition to considering the complex interaction between different species to preserve the integrity and biodiversity within the ecosystem.

3. Methods

Simulation software significantly contributes to the development of process design in academia and industry. They permit the development and evaluation of process designs with minimal effort and experimentation. In this work, we add to this characteristic by including the ecosystem services of carbon sequestration and air quality regulation provided by vegetation as unit operations. We use CHEMCAD to develop two unit operations for the restoration and plantation approaches and employ them to compare vegetation ecosystem services with technological solutions that perform the same function. The models and data sources used to develop the tools in this study are summarized in Fig. 1.

3.1. Vegetation unit operations

The capacity of vegetation to regulate air quality and sequester carbon depends on multiple factors such as the species, age, size, elevation, and location of the tree. This study uses data from the state-of-the-art United States Department of Agriculture (USDA) Forest Service software suite i-Tree (I-Tree, 2016). I-tree county is one of the available tools that estimates the benefits of trees in a county in the United States. This tool incorporates different models and processes to estimate the benefits from trees with high spatial resolution, including data for land cover, evergreen cover (USGS, 2015), weather (National Oceanic and Atmospheric Administration, 2022), leaf area index (Yang et al., 2006), air pollutant concentration (EPA, 2015), and population (U.S. Census Bureau, 2015). In addition, the model can estimate the amount of carbon stored and sequestered, vegetation uptake of pollutants, and the health impact cost in each county (Hirabayashi, 2016), as described in brief in this section.

The amount of carbon stored and sequestered was calculated based on the biomass growth equations using field collected data to determine the number of trees, species composition, stem diameter, tree height, crown width, tree cover percentage, and carbon densities per unit of tree cover (Nowak et al., 2013). In addition, carbon storage and sequestration were estimated for the nonforest land cover class using values and measurements from urban forests (Nowak et al., 2013). By contrast, forest carbon was estimated using the forest inventory and analysis data from the US Forest Service (Woudenberg et al., 2010).

The vegetation uptake or flux ($F_{i,j}$) of an air pollutant in county i was based on the dry deposition of pollutant j on trees as follows:

$$F_{i,j} = v^d_{i,j} \times C_{i,j} \times A_{v,i} \tag{1}$$

Here, ($v^d_{i,j}$) denotes the deposition velocity, ($C_{i,j}$) denotes the pollutant concentration, and ($A_{v,i}$) denotes the vegetation-covered area (Nowak et al., 2013). The concentration of each pollutant was obtained from the Air Quality System national database, US EPA (EPA, 2015). In addition, the hourly deposition velocity was calculated using local meteorological data from the National Climatic Data Center (National Oceanic and Atmospheric Administration, 2022).

Various variables, including tree spacing, age, location, and others, influence the required land area for a forest ecosystem. For this study, we used the i-tree parameter values as an average for each county. However, since land value does not depreciate, we only considered property tax as the annual land cost. The developed tool allows the user the option to input land costs for calculation purposes. If the land cost was unknown, we used the farm real estate average value per acre from the USDA (United States Department of Agriculture, 2022). Concerning the capital and maintenance costs for the forest ecosystem, we used the cost estimates from the Texas A&M Forest Service to determine the site preparation and annual maintenance costs (Texas A&M Forest Service, 2013).

Most software for simulating chemical processes includes a library of unit operations that represent a chemical process using current technological equipment. While they do not have any ecological alternative units, they allow the user to define their unit operation using custom models and equations. This is typically accomplished through a third-party medium that connects the new model to the software. We used the CHEMCAD simulation software with Microsoft Excel as the third-party medium to connect our vegetation models. CHEMCAD simulates the process flowsheet in a sequential and modular manner until it reaches the user-defined unit operation. Subsequently, it sends the stream data to the Excel sheet, where calculations are performed. The Excel sheet then sends the data back to CHEMCAD. As shown in Fig. 2, the vegetation model can be connected to other units in the simulation environment via input and output streams.

To utilize the models and data for the vegetation unit operation, the user must provide certain design parameters, such as the available land area and the design location. Correspondingly, the spatial information is requested using the county's Federal Information Processing System, which uses numbers uniquely identifying geographic areas. For the ecosystem restoration design approach, the tool automatically calculates the natural canopy cover percentage using the location and data from the national land cover database (USGS, 2015). For the plantation

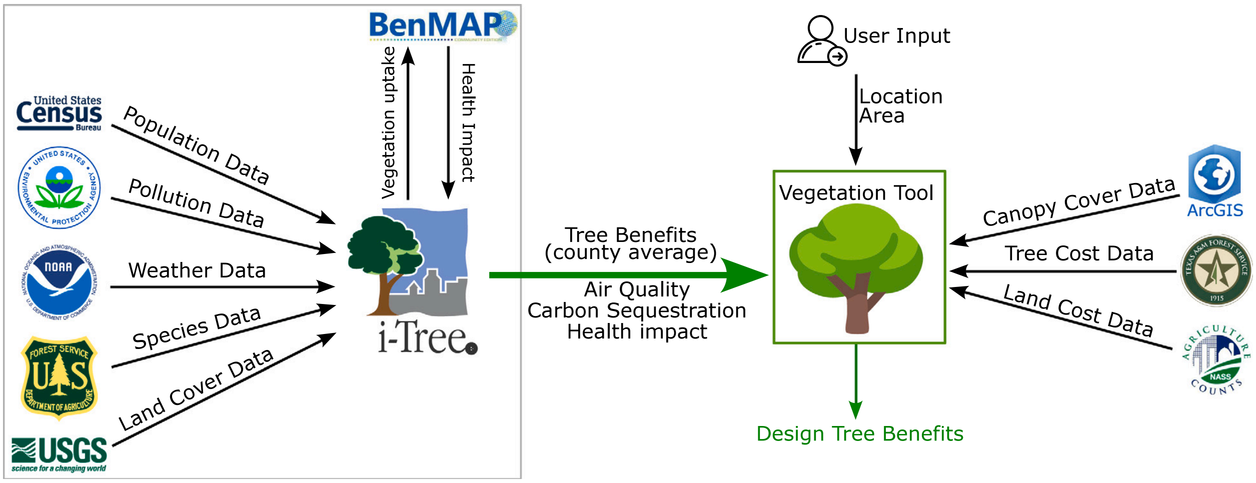

Fig. 1. Data sources used in the development of the vegetation tool.

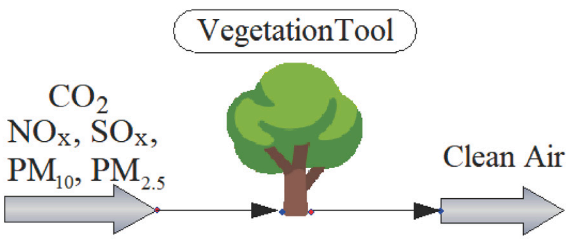

Fig. 2. Preview of the vegetation unit operation in CHEMCAD simulation environment.

approach, the user must specify the desired canopy cover percentage to calculate the benefits and removal capacities accurately.

Based on these inputs, the tools calculate the annual vegetation uptake of CO_2, NO_2, SO_2, $PM_{2.5}$, PM_{10} and O_3, as well as the health impact costs of the designed unit. However, to calculate the capital cost of the unit, the land cost per unit area must be known. Thus, the tools determined the cost based on the average land value in a county (United States Department of Agriculture, 2022) or based on the value provided by the user. As an additional feature, the units provide the design parameters and associated costs necessary to achieve net-zero impact goals, as depicted in Fig. 3.

To use the data provided by the i-tree county tool in chemical process design, we must calculate the uptake and benefits factors for each county using the original data. Since all the benefits provided by trees were dependent on the vegetated area ($A_{v,i}$) in a particular county, we utilized The National Land Cover Database (NLCD) (USGS, 2015) in the geographic information system software ArcGIS to determine the canopy cover percentage (α_i) in each county i. The NLCD divided the national land cover into nine classes and 20 subclasses: water, developed land, barren land, and forests. We follow the i-tree tool to calculate the canopy cover, considering only land classified as barren, forest, shrubland, herbaceous, planted and cultivated, and wetland classes. Consequently, we calculate the vegetated area as

$$A_{v,i} = A_{total,i} \times \alpha_i \tag{2}$$

Subsequently, the uptake factor ($f_{i,j}^{uptake}$) per unit area for the pollutant j is calculated as follows:

$$f_{i,j}^{uptake} = \frac{m_{i,j}^{total}}{A_{v,i}} \tag{3}$$

where, ($m_{i,j}^{total}$) is the total removal in (kg/year) retrieved from the i-tree tool.

Similarly, we calculate the health impact factors ($f_{i,j}^{health}$) using the information from the i-tree tool of the value of the total benefits ($V_{i,j}^{total}$) in ($/year) in a county divided by the total removal of pollutant j as follows:

$$f_{i,j}^{health} = \frac{V_{i,j}^{total}}{m_{i,j}^{total}} \tag{4}$$

In incorporating ecological alternatives into process design, multiple parameters must be considered, including the location of the process, the available land area, the vegetation cover, and the species of trees. Since the i-tree canopy provides benefits based on the species present in each county, we assume that the same species inhabit the design area. Subsequently, the total uptake capacity of the design area ($U_{i,j}^{design}$) in (kg/year) comprise the following:

$$U_{i,j}^{design} = f_{i,j}^{uptake} \times A_i^{design} \times \alpha_i^{design} \tag{5}$$

3.2. Technological unit operations

Current technological control strategies and equipment have been implemented to limit CO_2 and air-pollutant emissions from industrial processes. Engineered technological solutions are usually highly efficient because they are designed for a specific task. However, they include very expensive equipment with high operating and maintenance costs.

This study compares multiple ecosystem services obtained from trees with technological equipment that perform the same functions. To control the NO_x and SO_2 emissions, we consider selective catalytic reduction (SCR) and flue gas desulfurization (FGD) systems, respectively. Additionally, a baghouse filter is used to limit the release of particulate matter (PM). Finally, we consider a carbon-capture system to compare the carbon sequestration abilities of the vegetation ecosystem. Notably, current carbon-capture technologies require additional expense and energy to dehydrate, compress, transport, and store carbon after separating from flue gas. This step and its associated cost are not considered in this study. Consequently, this study underestimates the cost of technological carbon capture. Such information may be incorporated via additional unit operations for these steps.

The capital and operating cost equations for the SCR, a baghouse filter, and FGD were based on the EPA Air Pollution Control Cost Manual (Environmental Protection Agency, 2017). The unit cost of carbon capture was based on the US Energy Information Administration (EIA)34 report (EIA, 2020).

To ensure a fair comparison, all costs are expressed in the value of 2019 dollar, and the costs of the technological and ecological solutions

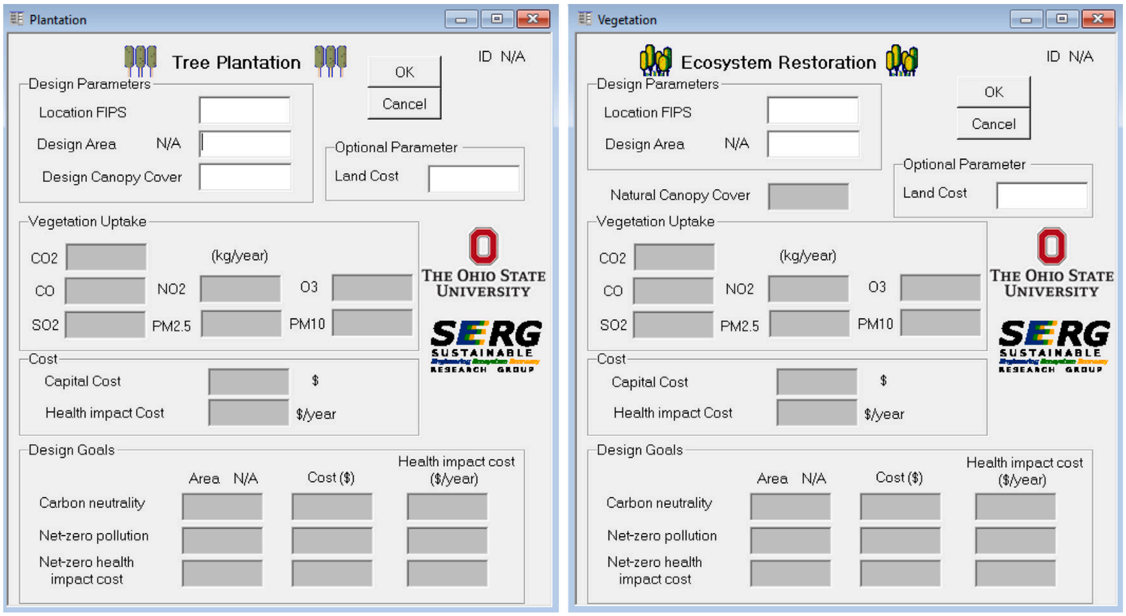

Fig. 3. User interface of the vegetation tool. The tools calculate the vegetation uptake and associated costs in the gray cells for the ecosystem restoration and plantation approaches. The restoration approach uses the natural canopy cover percentage in the county, while the plantation approach is based on user input and can be designed with a high canopy cover percentage. The white cells are user input information required for calculations such as the location, available land area, and canopy cover percentage. The tools also calculate the area necessary for the different design goals for the same location.

are converted to equivalent annualized cost (EAC) using the discount rate (r) and the project life span (n) as follows:

$$EAC = \frac{CapitalCost}{1-(1+r)^{-n}} \tag{6}$$

3.3. Health impact cost

The pollution uptake by vegetation considerably improves air quality and reduces the negative health effects on nearby communities. The US EPA Environmental Benefits Mapping and Analysis Program Community Edition (BenMAP-CE) model (US Environmental Protection Agency (USEPA), 2022) was used to estimate the health and monetary effects when the population experiences changes in air quality. The model starts with a base case containing the concentrations of various pollutants and then estimates the potential health incidence using multiple concentration–response functions and economic forecasting models (Nowak et al., 2013; US Environmental Protection Agency (USEPA), 2022). The functions were derived by calculating the change in the number of health effects (ΔY) due to a change in pollutant concentration (ΔC_j) using population size (P), an effect coefficient from epidemiological studies (β), and a baseline incidence rate (Y_0) of the health effect, as described in the BenMAP user manual (US Environmental Protection Agency (USEPA), 2022). One of the functions used by BenMAP to estimate the health impact of a change in PM_{10} concentration is below as an example.

$$\Delta Y = f(\Delta C_j, P, \beta, Y_0) \tag{7}$$

$$\Delta Y = Y_0 \times (1 - e^{-\beta \Delta C_{PM_{10}}}) \times P \tag{8}$$

After estimating the health incidents due to a change in a pollutant concentration, the BenMAP-CE model was used to calculate the health benefits of trees' uptake of pollutants. Subsequently, the economic valuation of the change in health incidence was estimated using multiple valuation functions, such as willingness to pay, Cost of Illness, and Value of Statistical Life (US Environmental Protection Agency (USEPA), 2022). These functions estimate the value of direct and indirect effects, such as medical costs and missing time at work, respectively. Finally, the total valuation is calculated by multiplying the estimated number of adverse health effects by one of the valuation functions.

$$\text{Health impact benefits} = \text{Number of cases} \times \text{Valuation function} \tag{9}$$

3.4. Design approaches and goals

As mentioned in Section 2.2, two approaches are available for designing a vegetation ecosystem: tree plantation and ecosystem restoration. Based on the canopy cover input by the user and the natural canopy cover, the tools developed herein were used to calculate the results for the plantation approach and the restoration approach, respectively. Because most landscapes have been altered through human development and activities, the current canopy cover percentages do not reflect the natural state of the vegetation ecosystem. Therefore, we must determine the actual canopy cover (α_i^a) in each county when considering the ecosystem restoration approach. We use ArcGIS to find different land cover classes in each county using the data from the NLCD (USGS, 2015). Subsequently, we eliminate the developed areas and the water-covered areas to determine the actual natural canopy cover as follows:

$$\alpha_i^a = \frac{A_{v,i}}{A_{total,i} - A_{water,i} - A_{developed,i}} \tag{10}$$

Depending on land area, environmental conditions, and budget, the ecological solution to mitigate air pollution and carbon sequestration can be designed in various ways. Herein, we defined three goals to assist decision makers in analyzing the benefits of the vegetation unit operation:

Carbon Neutrality:

Attaining net-zero CO_2 emissions has been one of the most sought-after goals for countries and corporations attempting to address environmental challenges such as global warming. This goal ensures that the amount of CO_2 sequestered by vegetation in the design is equal to or greater than the amount of CO_2 emitted by the process ($m_{i,CO_2}^{Process}$). Thus, the minimum design area with a known percentage of canopy cover is calculated as follows:

$$A_i^{design} = \frac{m_{i,CO_2}^{Process}}{\alpha_i^{design} \times f_{i,CO_2}^{uptake}} \tag{11}$$

Net-zero Pollution:

Regulating criteria air pollutants can be both economically and socially expensive. Typically, the capital and maintenance costs for technological equipment that limit the release of air pollutants are quite high. Moreover, air pollutants are the leading cause of health issues in neighboring communities. Therefore, this design goal aims to identify the area required to uptake all the pollutants that a process emits. Consequently, the land area was found to vary considerably based on the location of the process and the background concentration of pollutants. Thus, to determine the land area required to achieve net-zero pollution, we first determined the area required to remove each pollutant j, then selected the largest area.

$$A_i^{design} = \max_j\left(\frac{m_{i,j}^{Process}}{\alpha_i^{design} \times f_{i,j}^{uptake}}\right) \tag{12}$$

Notably, net-zero pollution for the vegetation ecosystem is not the same as zero pollution with technological equipment. With technology, no pollutants will be released into the environment, which can result in zero impact. However, vegetation will remove pollutants over time to reach the net-zero goal. Therefore, if we rely on nature, pollutants will have some impact on society and the environment initially.

Net-zero Health Impact Cost

The health impact cost of air pollution varies greatly depending on the location of the process, population, and background concentration of the pollutant. Consequently, the health impact factor for each pollutant will vary based on the study area. This design goal finds the land area of vegetation required for a net-zero social health impact cost. Correspondingly, this goal is likely to prioritize benefits by prioritizing the most expensive pollutant, even if the process does not release a significant amount. The design land area is calculated as follows:

$$A_i^{design} = \frac{\Sigma(m_{i,j}^{Process} \times f_{i,j}^{health})}{\Sigma(f_{i,j}^{uptake} \times f_{i,j}^{health})} \div \alpha_i^{design} \tag{13}$$

4. Case study

4.1. Power plant

To test and demonstrate the practicality of the vegetation tool, we consider a typical energy power system design. This example is quite general and an essential part of any chemical manufacturing facility. We simulate an on-site small-scale coal-fired power plant that provides electricity and steam for a manufacturing process. The power plant has a capacity of 0.8 MW and is designed to generate a net power of 7000 MWh/year with 60% efficiency. The addition of control equipment will result in a larger unit size to compensate for the additional auxiliary load requirements. Hence, the net power generation basis will provide a meaningful comparison between the scenarios with different control equipment. We use a discount rate of 7% and a project life span of 30 years for calculating the equivalent annualized cost (EAC). The plant investigated in this study was assumed to be located in Hamilton County, Ohio. However, as described in Section 5.2, we also consider other locations across the country.

Coal burning produces CO_2 and air pollutants, such as SO_2, NO_x, PM. The local Pittsburgh No. 8 bituminous coal is assumed to be the fuel used in the power plant, with the composition and heating values (Summers, 2019; The Code of Federal Regulations, 2022) shown in Table 1. The coal has a moisture content of 2.63%, a high ash content of 9.17%, and a sulfur content of 1.46%.

Fig. 4 shows the flowsheet of the power plant in the simulation environment, with control units including the vegetation unit operation. The CHEMCAD simulation software is used herein to model and simulate the process and different scenarios. The design parameters, energy requirements, and economic costs are based on the optimized and detailed design of the National Energy Technology Laboratory report (Robert et al., 2019) for fossil energy plants.

Table 1
Composition and heating values of coal (Pittsburgh No. 8).

	%
Moisture	2.63
Ash	9.17
Carbon	73.15
Hydrogen	4.97
Oxygen	6.22
Nitrogen	2.36
Chlorine	0.04
Sulfur	1.46
HHV (kJ/kg)	28 970

After the coal burning process, the flue gas is first sent to an SCR to control NO_x emissions. The SCR uses Ammonia (NH_3) and a catalyst to reduce NO_x emissions into nitrogen and water with 90% efficiency (Environmental Protection Agency, 2017). Then, the flue gas passes through a baghouse filter to limit the release of PM, with 99% efficiency. The baghouse filter is designed with a gas-to-cloth ratio of 0.762 m/min using 5-1/8-inch glass fiber bags. Other parameters, such as the number of bags, cages, and fabric area, vary based on unit size and flue gas flow rate (Environmental Protection Agency, 2017).

Subsequently, a wet limestone scrubber is used as an FGD system, with a standard efficiency of 98%, to control SO_2 emissions (Environmental Protection Agency, 2017). Finally, the flue gas is sent to a monoethanolamine (MEA) based carbon-capture system with a 90% carbon removal rate (Environmental Protection Agency, 2017). After passing through a direct contact cooler, the flue gas enters an absorber, where CO_2 reacts with the absorbent to form a CO_2-rich amine that is then sent to the stripper for separation.

We estimate the land required for a power plant, including the control equipment, based on the total energy generation in the United States and the land use for the power plant, as reported by EIA and the Natural Gas Supply Association (Natural Gas Supply Association, 2022; Stevens et al., 2017).

4.2. Scenarios

Comparison of the different scenarios is crucial for assessment and decision making in the design process. Moreover, the tradeoffs between meeting energy demand, regulating emissions, and preventing any societal impact provide perspectives to policy and decision makers. Therefore, we considered different designs using different control strategies to study the economic, environmental, and social effects of incorporating ecosystems into the process design, as detailed in Fig. 5 and Table 2.

In scenario A, we focus only on minimizing the economic cost to the company and simulate the power generation system without any control equipment. In scenario B, we add the technological control equipment with their standard removal efficiencies, including SCR, a baghouse filter, FGD, and carbon capture. Subsequently, we simulate the power plant with the vegetation ecosystem as the control strategy using the tools developed for the plantation (scenario C1) with a 90% canopy cover and ecosystem restoration (scenario C2) with the actual canopy cover for Hamilton County, Ohio (39.71%) (USGS, 2015). In Scenario C, we assume that the local emissions from the power plant are insufficient to cause substantial damage that inhibits tree growth and function or causes tree death.

Due to technological limitations, the control equipment could not eliminate 100% of the power plant emissions. Therefore, scenarios D1 and D2 include vegetation to remove the power plant emissions not captured by technological equipment.

Lastly, scenarios E1 and E2 investigate the effect of integrating the uptake capacities of vegetation into the design and evaluate the performance and cost of the power plant based on varying proportions of flue gas treatment by vegetation and technology.

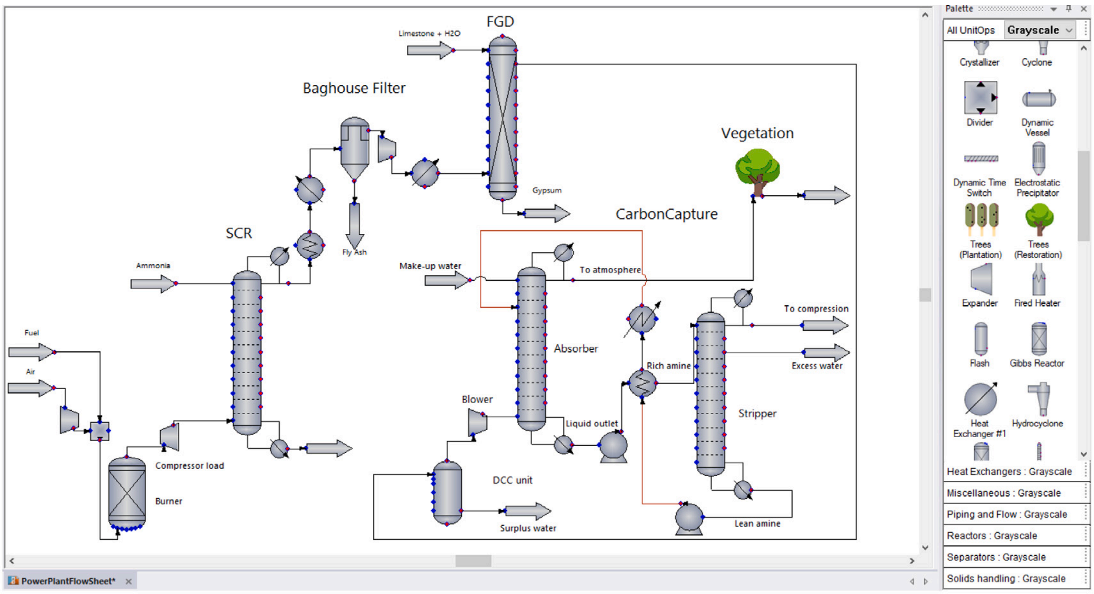

Fig. 4. Flowsheet showing different sections and units for the energy power plant including the control equipment and the vegetation unit.

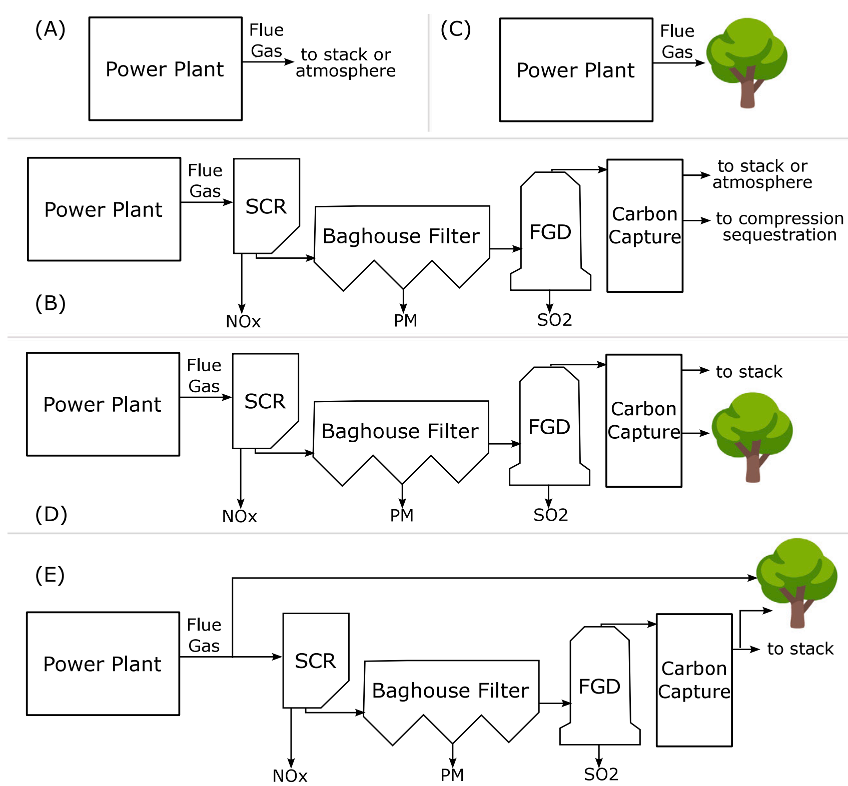

Fig. 5. Schematic showing the different scenarios and control alternatives. In scenario A, the flue gas is released into the environment without any control equipment. Scenario B uses technological equipment to control most air pollutants and carbon emissions. The design in scenario C utilizes vegetation to remove air pollutants and sequester the carbon released to the environment. A combination of the control solutions is evaluated where the vegetation is used to remove the remaining emissions after it goes through the standard technological equipment in scenario D. Scenario E evaluates an integrated design where the uptake capacity of the vegetation is considered in the design of the plant along the technological equipment.

5. Results

The simulation results of the coal-fired power plant to achieve the required net generation indicate that the flue gas contains a substantial proportion of CO_2 and air pollutants. The composition and flow rate of flue gas is detailed in Table 3.

Introducing control equipment will necessitate a larger generation unit, and consequently, the total emissions will likely increase accordingly. Fig. 6 depicts a comparison between the cost to company and the health impact cost for scenarios A, B, C1, and C2. As observed in scenario A, the lowest cost to the company corresponds to not having any control equipment. At the same time, it is the scenario with the

Table 2
Simulation scenarios to control the emissions from the power plant.

Scenario	Control	Design
A	No control	Only power generation
B	Technology	High efficiency control equipment
C1	Vegetation (Plantation)	Trees to uptake emissions and air pollutants
C2	Vegetation (Restoration)	
D1	Technology + Vegetation (Plantation)	Technological equipment + Trees to remove the remaining emissions
D2	Technology + Vegetation (Restoration)	
E1	Technology + Vegetation (Plantation)	Integrated Design: Flue gas is split between technology and vegetation
E2	Technology + Vegetation (Restoration)	

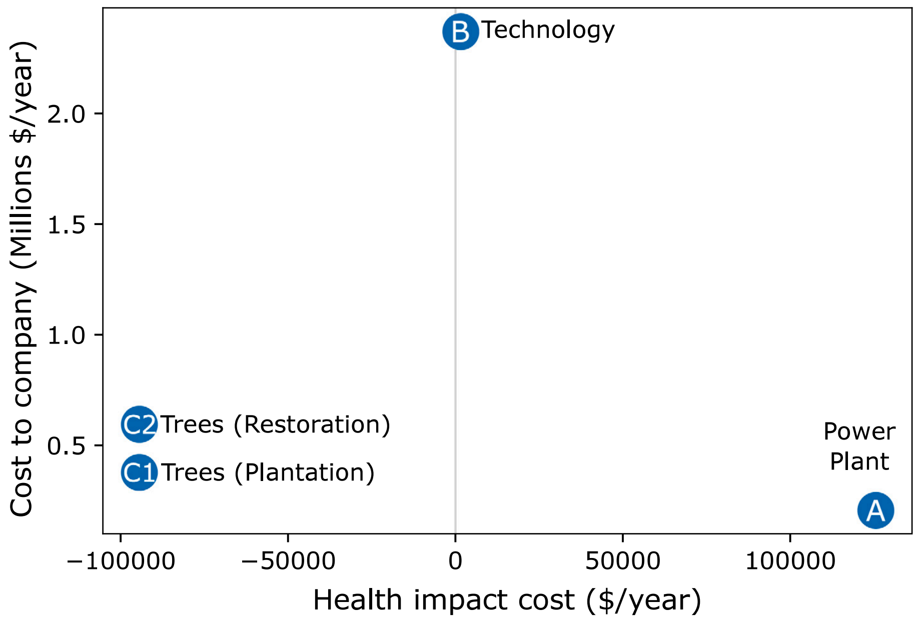

Fig. 6. Economic and health impact cost comparison using technology and trees as control strategies for the power plant.

Table 3
Flue gas composition.

	kg/year
CO_2	2 230 427
NO_2	1432
SO_2	2170
PM_{10}	917
$PM_{2.5}$	994

highest health impact cost resulting from uncontrolled emissions. The addition of control equipment (scenario B) has a noticeable effect on reducing the health impact and increasing the economic cost of the company.

Utilizing trees to mitigate all emissions (scenarios C1 and C2) offers attractive solutions, as the health impact cost is reduced, and the economic cost is very low. However, tree uptake occurs over time; thus, relying solely on trees will release pollutants into the environment and impact local communities. In addition, based on the employed reforestation strategy, a vast area of land will be necessary for trees to mitigate the emissions from the power plant.

To assess and evaluate the addition of vegetation to supplement the control equipment, we use trees to mitigate the remaining emissions from the power plant. We use the developed CHEMCAD tool to design the vegetation to achieve one of the net-zero impact goals discussed in Section 3.4. In addition, we investigate the impact of these designs when the removal efficiency of the technological equipment mentioned in Section 4.1 decreases.

In Fig. 7, we compare the cost to company and health impact cost of scenario B to scenarios D1 and D2 for the goals of net-zero carbon emissions and net-zero pollution. The results are presented as curves beginning with the efficiency of the equipment in the base case, followed by the cases in which the efficiency is reduced by 1% to 5%. As observed, the use of technology alone always negatively impacts health impact cost which increases as efficiency decreases. Conversely, adding trees considerably decreases the health impact cost, resulting in a net negative cost or benefit. However, due to the need for a larger vegetation system, there is a slight increase in the design expense as a result of the decreased efficiency. As expected from an engineered system, the results indicate plantation-based designs are less expensive than ecosystem restoration approaches. Notably, the indirect health impact cost of carbon was not considered in this work. This expense represents the consequences of climate change due to the increased atmospheric carbon dioxide concentration. The health impact cost includes the mortalities from extreme heat, extreme weather events, the impact on food and water supplies, and an increase in disease and aeroallergens. We expect these results to change dramatically when we consider the additional ecosystem services vegetation provides, which will favor the restoration approach.

5.1. Techno-ecological synergies for integrated designs

It is evident from the results of the previous scenarios described in Section 5 that there are tradeoffs between technological and ecological solutions for carbon sequestration and pollution regulations. Technology excels in terms of high efficiency and small land requirements. Meanwhile, the vegetation ecosystem is superior in terms of low cost to the company and lower health impact, although it requires a large land area. These characteristics can be utilized to create a synergistic design

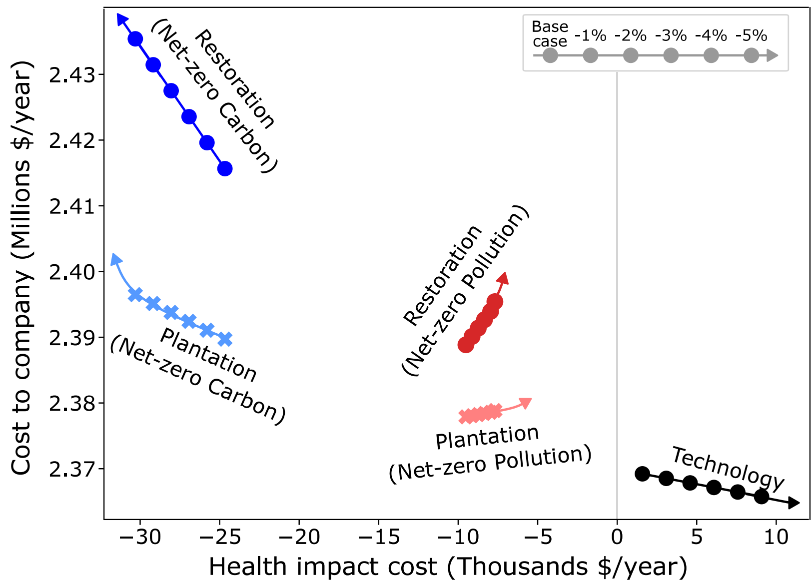

Fig. 7. The advantage of including vegetation for emission removal with decreasing efficiency of technological equipment in terms of cost to company and health impact cost. The dots in each curve represent a simulation with standard efficiency followed by less efficient equipment with a 1% decrement. The results show that technology alone cannot achieve net-zero carbon or net-zero pollution. Further, the results show a significant reduction in the health impact cost for all reforestation approaches and design goals.

that combines the benefits of both solutions. In addition, since the majority of technological control equipment is designed with standard removal rates, their capital costs and energy demands largely depend on the flue gas flow rate. Therefore, by reducing the flue gas flow rate to the technological equipment and redirecting it to the ecological system, the size and emissions of the power plant will decrease due to the reduced auxiliary and energy requirements of the equipment. Using this information, we identify various combinations of solutions that utilize the advantageous aspects of both control strategies.

Fig. 8 depicts the integrated design results for scenarios E1 and E2 with varying treatment percentages for different design goals. Starting with the technology-only solution (full gray circle, scenario B), we can observe an increasing improvement in the health impact cost by adapting more ecological solutions. Designing the ecological system using the plantation approach reveals numerous configurations with “win-win” solutions that reduce the cost to the company and the health impact cost. The approach to restoring ecosystems results in a similar improvement in the health impact cost while incurring minimal additional expenses for the company. Similar to scenarios D1 and D2, we anticipate that the cost to the company will decrease as a result of the additional services provided by the vegetation ecosystem. Notably, by suggesting that trees produce better economic and social outcomes, we are not promoting the release of pollutants into the atmosphere. Government agencies continue to require power plants to comply with their emissions regulations. Thus, we are highlighting the tradeoffs and capabilities of trees to mitigate emissions to comprehend the interaction between technological and ecological systems, and develop synergistic designs based on this knowledge. These designs can go beyond merely complying with regulations and enable businesses to meet the increasingly prevalent goals of nature-positive and people-positive decisions (Obura et al., 2023).

5.2. Vegetation as a solution across diverse landscapes

All the results presented so far were for a power plant in Hamilton County, Ohio. These results will considerably vary if the power plant is in a different county. This is due to the spatial variation of the vegetation ecosystem, including the uptake capacities of prevalent local tree species and the background concentration of a specific pollutant. We simulated the power plant using the exact flue gas specifications listed in Table 3 to study the effect of the spatial information. We compared the results for Hamilton County, Ohio, to the results obtained for Washington County, Mississippi, and Pima County, Arizona, because their ecological and economic characteristics differ considerably, as summarized in Table 4.

Fig. 9 depicts the simulation results for land requirements and the annual cost to the company to achieve different net-zero impact goals. The results presented in this study for the carbon-sink plantation strategy were not simulated based on monoculture or near-monoculture plantation projects. Instead, we used the average tree species in each county with a very high canopy cover percentage. This assumption was made due to the high variation in the uptake capacity of different tree species that can be utilized in different plantation projects. As observed, Washington County has the lowest cost and land area requirements to achieve carbon neutrality using the carbon-sink plantation approach. However, Washington County requires a larger land area than Hamilton County if the ecosystem restoration strategy is implemented. Nevertheless, the total cost of the power plant to the company is lower in Washington County. Although native tree species in Washington County have a high uptake capacity, the difference in area requirements between the two reforestation strategies results from land use change. Currently, more than 70% of the land in the county is devoted to crop cultivation. In this comparison, we did not consider any tax exemptions that might be available for different states or counties.

It is not surprising that Pima County has the largest area requirement because it has the lowest canopy cover and uptake capacity. However, when using the plantation approach, Pima County has the smallest area requirement to achieve net-zero health impact cost owing to the high benefits of removing air pollutants such as SO_2 and $PM_{2.5}$ from the county. For this case study, highest land area and cost are required for achieving the goal of net-zero pollution in case of both reforestation approaches. This is due to the limited uptake capacity for certain pollutants in different counties. For example, compared with the removal of all other pollutants, removing SO_2 required the largest land area in Washington and Pima counties, while $PM_{2.5}$ had the highest land area requirements in Hamilton County.

This spatial variation identifies a “limiting pollutant” or the lowest vegetation uptake factor for each county in the United States as follows:

$$\text{limiting pollutant}_i = \min f_{i,j}^{uptake} \qquad \forall j \tag{14}$$

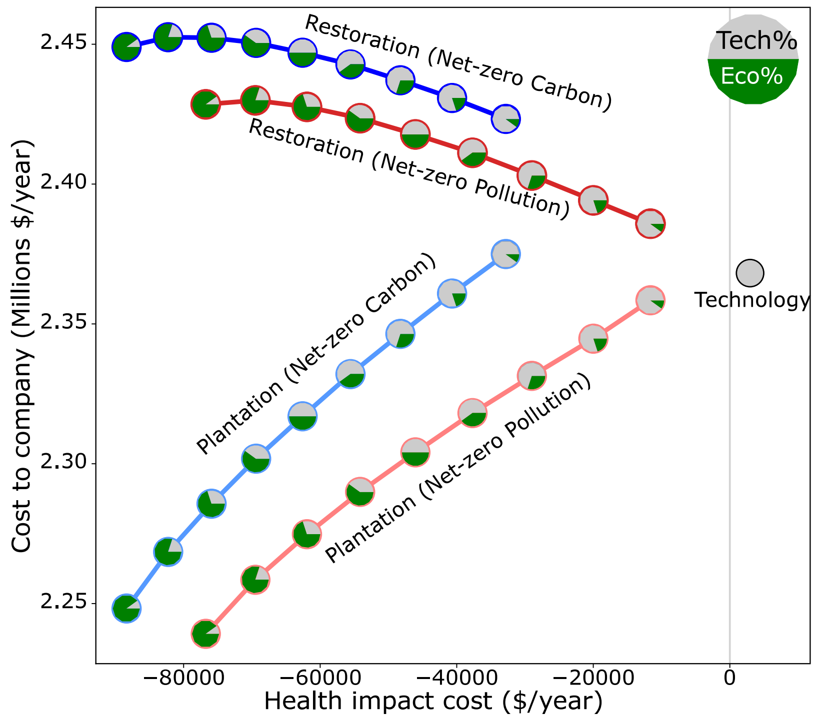

Fig. 8. The trade-off between economic and health impact cost for the integrated design. The pie charts show the fraction of where the flue gas is treated. Even a minimal utilization of vegetation yields a significant improvement in the health impact cost. Using the tree plantation approach can yield multiple "win-win" solutions.

Table 4
Ecological and economic characteristics for selected counties.

County	Actual canopy cover (%)	Land cost ($/acre) (United States Department of Agriculture, 2022)	Annual O&M cost ($/acre/yr) (Texas A&M Forest Service, 2013)
Hamilton, OH	39.71	6290	190
Washington, MS	13.88	2800	115
Pima, AZ	0.51	3800	117

For the design of processes, systems, or supply chains, it is crucial to comprehend the current conditions and limitations of vegetation uptake capacities in various locations. Without accounting for the limiting pollutant, designing a vegetation ecosystem or considering a synergistic design with technology may result in poor performance and high costs. For instance, if a chemical process has high SO_2 emissions, decision makers should avoid designing in counties where SO_2 is the limiting pollutant. Fig. 10 depicts the limiting pollutant for counties across the United States.

However, as described in Table 3, for our calculation and design, the limiting pollutant is also a factor in the flow rate of pollutants from the power plant. Combining the uptake factor and the amount of pollutant in land area calculations presents an intriguing spatial information problem. As depicted in Fig. 11, we performed the simulation across the counties of the United States for the different goals of scenarios C1 and C2. The grayed-out counties indicate solutions where the required land is either greater than the county's total area or exceeds 5000 acres.

6. Conclusions

This study highlights the potential benefits of including vegetation ecosystems into the design of chemical processes. The inclusion is demonstrated by designing unit operation modules used in the simulation software. We evaluate the carbon sequestration and air quality regulation services of the vegetation ecosystem and compare them to the technological control standards used in the industry. The combination of these two control options results in a synergistic design that reduces social and economic costs.

For the case study of a power plant highlighted in this work, we observe that including vegetation is essential for mitigating the costs associated with health impacts. Using vegetation instead of technological control equipment can be incredibly cost-effective when sufficient land area is available. Meanwhile, if the designed land area is limited, the combination of technological and ecological solutions can be very attractive.

This study identifies the ability of the vegetation ecosystem to sequester carbon and remove air pollutants by including detailed models with spatial information through the developed tools. We compare two approaches for vegetation in our models and observe that tree plantation exhibits a higher carbon sequestration rate than ecosystem restoration. However, tree plantations are less resilient than ecosystem restoration, are more likely to negatively impact other natural ecosystems, require greater human intervention, and provide fewer ecosystem services. Many uncertainties come with data and models from different sources like the ones presented in this work. We have used the most recent and accurate data available from reliable sources to reduce these uncertainties. Although this study does not consider the dynamics of ecosystems, it uses the annual average values as a design estimate. In addition, we use average parameters in each county, such as tree species and age, assuming that the user does not have this information. The use of more advanced models is encouraged to obtain more accurate results.

The generality of the developed tools will enable more exploration of new integrated designs for various applications. The tools suggest different designs based on goals, such as carbon neutrality, net-zero pollution, and net-zero health impact cost. Different alternatives are

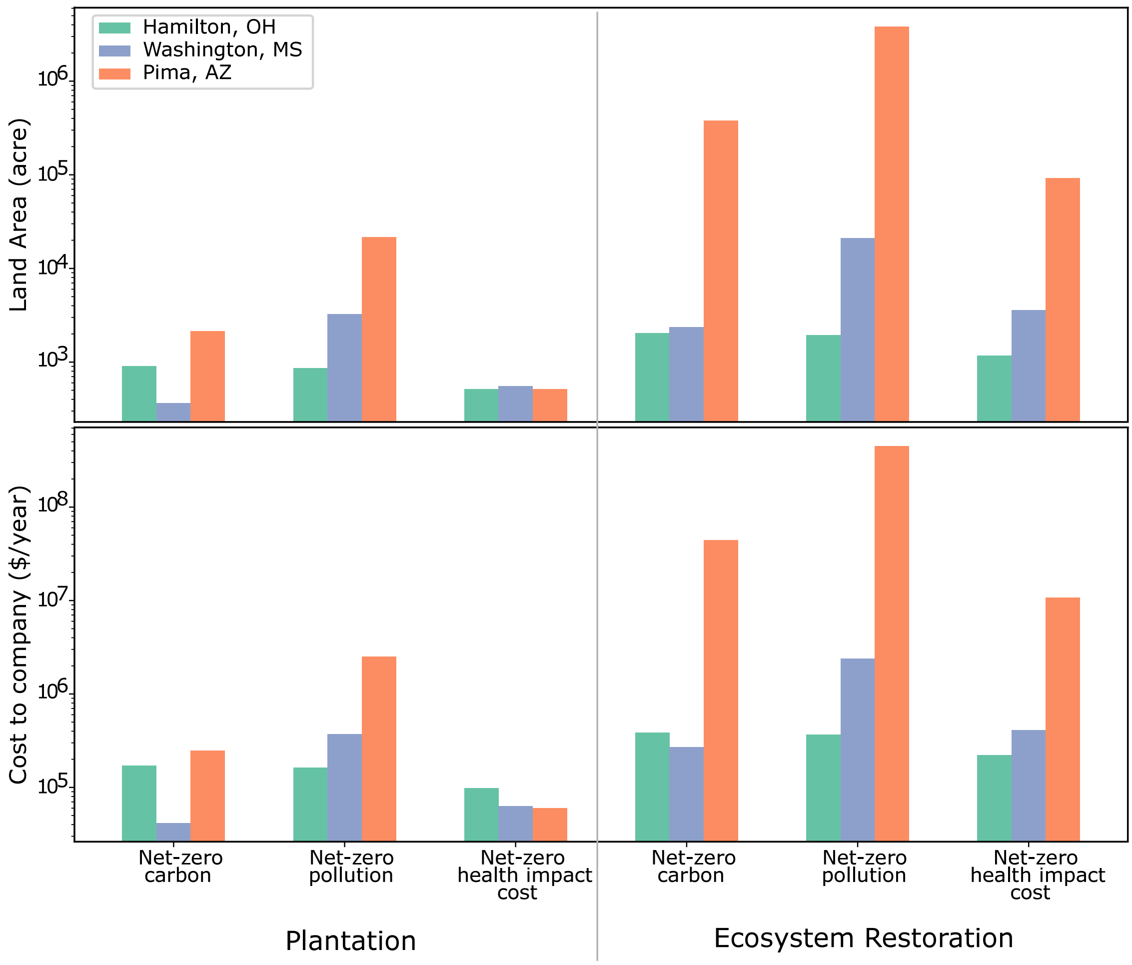

Fig. 9. The cost and land requirements to mitigate the emissions of the power plant. The results show that the plantation approach yields better results in terms of smaller land area and cost to company as a direct result of the higher canopy cover compared to the natural canopy cover in the ecosystem restoration approach. The results also highlight the importance of the plant's location that determines the land requirement, health impact cost, and cost to company, which depends on local factors such as the concentration of pollutants and uptake capacities of local vegetation.

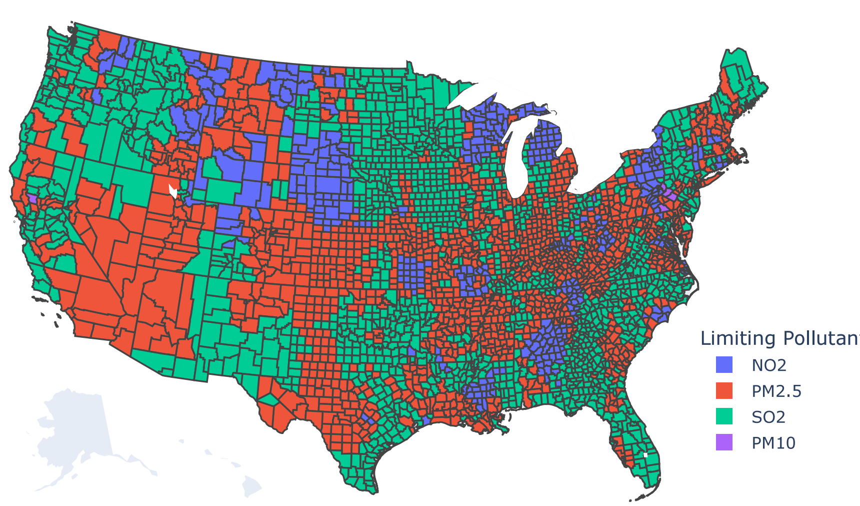

Fig. 10. Vegetation Limiting pollutant. This map identifies the pollutant in each county where the vegetation has the lowest capacity to remove based on tree species and the background concentration of that pollutant.

essential in aiding the decision-making process to achieve multiple goals. The tool can also facilitate complex optimization problems that involve finding potential location (Charles and Bakshi, 2021), tree species relating to chemical processes, to reduce air pollution. The emissions and health impact evaluated in this work is the process's direct impact and not the process's life cycle impact. Since traditional

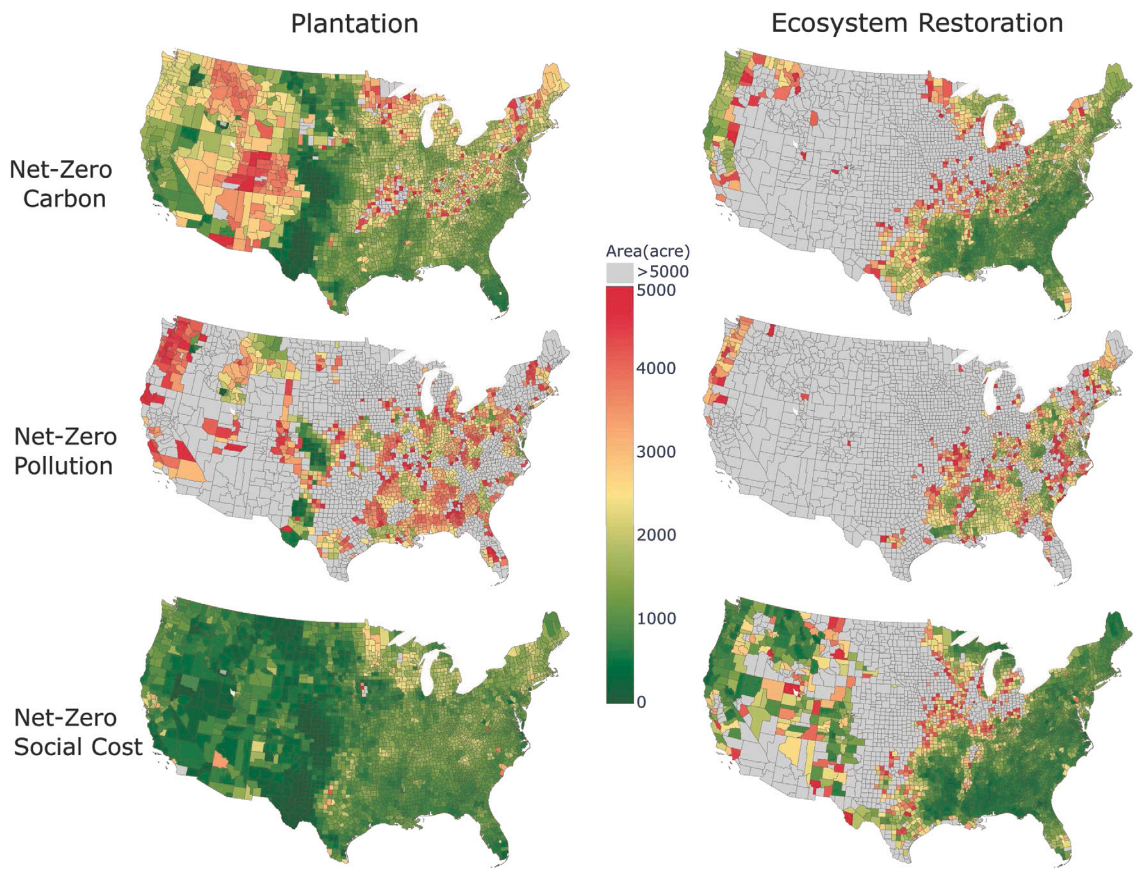

Fig. 11. Effect of plant location on land area requirements for Net-Zero impact goals. The color represents the land area needed to remove emissions from the plant. The gray-colored counties require a land area of more than 5000 acres or do not have enough land area to remove all the emissions. The results show that the plantation approach provides designs with fewer area requirements than the ecosystem restoration approach. However, the dominance of the gray-colored counties suggests that trees alone are inadequate and synergistic use with technologies may be considered.

design decisions are made on the equipment scale, the tools were also designed at the equipment scale. Although to reach the goal of sustainability, the life cycle impact of the process should be considered in the design process, but the simulation environments and tools are not at the life cycle scale yet.

This study strengthens the foundation of sustainable process design by incorporating ecosystems during the decision-making step of design, resulting in mutual benefits for society and nature. Incorporating vegetation as unit operation paves the way for other negative emission technologies, such as direct air capture, to be designed as unit operation and subsequently implemented in process design. However, further studies to include other ecosystems are necessary to understand the magnitude of the impact of industrial processes and find synergies to reduce stress and protect ecosystems.

CRediT authorship contribution statement

Yazeed M. Aleissa: Conceptualization, Methodology, Software, Investigation, Data curation, Writing – original draft, Writing – review & editing. **Bhavik R. Bakshi:** Conceptualization, Methodology, Resources, Writing – review & editing, Supervision, Project management.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The tool and the required files are provided via Zonodo data (Aleissa and Bakshi, 2023). https://doi.org/10.5281/zenodo.7387087.

Acknowledgment

Partial funding for this work was provided by King Abdulaziz University, Jeddah, Saudi Arabia through the sponsorship of Yazeed Aleissa.

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