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Techno-ecologically synergistic food–energy–water systems can meet human and ecosystem needs†

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Sustainable provisioning of energy to society requires consideration of the nexus between food–energy–water (FEW) flows while meeting human needs and respecting nature's capacity to provide goods and services. In this work, we explore the FEW nexus of conventional and techno-ecologically synergistic (TES) systems by evaluating combinations of various technological, agricultural, and ecological strategies from the viewpoints of electricity generation, food production, life cycle water use, carbon footprint, nutrient runoff, corporate profitability, and societal well-being. We evaluate activities related to power generation (coal and gas extraction and use, transportation options, cooling technologies, solar panels, wind turbines), food production (farming with and without tillage), waste utilization (carbon dioxide capture and conversion to hydrocarbons, green hydrogen), and ecological restoration (forests and wetlands). Application of this framework to the Muskingum River watershed in Ohio, U.S.A. indicates that seeking synergies between human and natural systems can provide innovative solutions that improve the FEW nexus while making positive contributions to society with greater respect for nature's limits. We show that the conventional engineering approach of relying only on technological approaches for meeting sustainability objectives can have limited environmental and societal benefits while reducing profitability. In contrast, techno-ecologically synergistic design between agricultural systems and wetlands can reduce nutrient runoff with little compromise in other goals. Additional synergies between farming and photovoltaic systems along with the use of wetlands can further improve the FEW nexus while reducing CO_2 and nutrient emissions, with a relatively small compromise in corporate profitability. These results should motivate further work on innovative TES designs that can provide "win–win" solutions for meeting global energy needs in an environmentally and socially beneficial manner.

Broader context

Preventing burden shifting and unintended side effects of energy provisioning technologies on the environment and society requires consideration of the nexus between food, energy, and water (FEW) flows. Unfortunately, most frameworks for assessing the FEW nexus of energy and other systems do not account for the role of ecosystems in sustaining human activities, and ignore the need to respect nature's limits. Such ignorance can contribute to ecological degradation and resource depletion and result in lost opportunities for developing innovative solutions for meeting society's energy needs by seeking synergies between technological and ecological systems. In this paper, we develop a framework for evaluating many combinations of alternatives for meeting FEW needs while paying attention to societal damages, corporate profitability, and nature's capacity to absorb carbon dioxide and nutrient runoff. A case study investigates various strategies for power generation, food production, waste utilization, and ecological restoration in the Muskingum River watershed in Ohio, U.S.A. We find that synergistic design of energy technologies such as solar panels with agricultural and ecological options can provide attractive solutions for meeting societal needs while respecting ecological constraints and contributing to human well-being.

1 Introduction

Ensuring the provisioning of energy while protecting the environment requires approaches for reducing the chance of burden shifting between food–energy–water (FEW) flows.[1,2] In addition to protecting the environment, economic feasibility, and societal desirability are also essential for sustainability of energy activities. More specifically, the demand for ecosystem services from human activities and the capacity of ecosystems to supply these services also need to be considered, since

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ecosystem flows interact with FEW flows.[3] For example, water supply is an abiotic ecosystem provisioning service[4] that is necessary to sustain the productivity of FEW systems such as agriculture and electricity generation. Also, by using resources and releasing wastes, FEW systems impact many ecosystem services such as regulation of climate, and air, water, and soil quality. Sustainability requires recognition of the fact that the supply of ecosystem services is finite, and therefore, nature's capacity must be respected to sustain the productivity of FEW systems[3] and prevent ecological degradation by staying within the safe operating space.[5] Simultaneous consideration of the demand and supply of ecosystem services can also help in discovering novel and innovative opportunities for mutually beneficial synergies between human and natural systems. Such techno-ecological synergies (TES)[6] encourage simultaneous and integrated improvement of technologies to meet human needs along with restoration and protection of ecosystems. TES designs can also be environmentally friendlier and economically superior to the techno-centric solutions developed by traditional engineering.[7–10]

Previous studies that considered ecosystem services with the FEW nexus either only addressed the water provisioning service[11–13] or did not perform quantitative work.[13–15] However, since ecosystem services interact with each other and are available as packages,[16] we need to account for multiple services simultaneously. For instance, forests provide the service of climate regulation but affect the freshwater provisioning service as well. Hanes *et al.* (2018)[3] addressed the nexus of local FEW systems, which include biomass conversion and land-use options, while quantitatively accounting for various ecosystem services. However, they did not consider the spatial scale of ecosystem services (*i.e.*, serviceshed), which is needed to gain insights into ecological overshoot and absolute sustainability.[17] The study also did not consider technological systems, which can be dominant activities due to their important role in meeting human needs and causing environmental impacts.

The watershed scale is suitable for addressing the FEW nexus since water is one of the primary resources for the food and energy sectors. In a watershed, common resources such as water and other ecosystem services support multiple human activities such as agriculture and industry. For the management of FEW systems, therefore, the watershed resources should be distributed sustainably among multilateral stakeholders.[18] Management plans must enhance the net gain of FEW systems while sustaining human communities as well as staying within ecological limits. Such needs are also being recognized by industry, as conveyed in the Business Roundtable's commitment to promoting benefits to all stakeholders, not just to shareholders.[19] However, systematic approaches to assess and design strategies to provide mutual benefits to multiple stakeholders are not yet available.

This work represents steps toward a much-needed transformation of the engineering paradigm from one that takes nature for granted to one that accounts for its role and respects its limits. The main contribution is to show that seeking synergies between human and natural systems can simultaneously improve the FEW nexus, make positive contributions to society, and reduce the transgression of nature's limits. We demonstrate this by developing a framework for techno-ecologically synergistic FEW (TES-FEW) nexus modeling and assessment, which allows us to understand the interactions between FEW systems, the waste they generate, and their dependence on ecosystems. Then, we discuss the environmental effectiveness and economic feasibility of various strategies from multiple perspectives (technological, agricultural, and ecological) to improve the watershed-scale sustainability of FEW systems. These strategies include approaches for mitigating nutrient pollution, CO_2 conversion, and emerging approaches for solar energy production. We demonstrate the benefits of TES design by applying our framework to activities in the Muskingum River Watershed (MRW) in Ohio, U.S.A. Accounting for nature's limits identifies additional opportunities toward sustainability by emphasizing the benefits of ecosystems.

2 Methods

2.1 Framework for techno-ecologically synergistic FEW nexus

The traditional FEW nexus framework mainly focuses on the interactions between FEW flows.[1] In this work, we develop a TES-FEW nexus framework by including ecosystem and waste flows as additional components to the nexus, as shown in Fig. 1. Ecosystems provide various benefits such as provisioning and regulating services to food and energy systems. If the environmental interventions of FEW systems such as water consumption and waste emissions exceed the corresponding supply of ecosystem services, as shown by blue and gray arrows in the figure, there will be ecological overshoot, which will lead to resource depletion and ecosystem degradation. Sustainability requires respect for nature's limits over a selected time period.

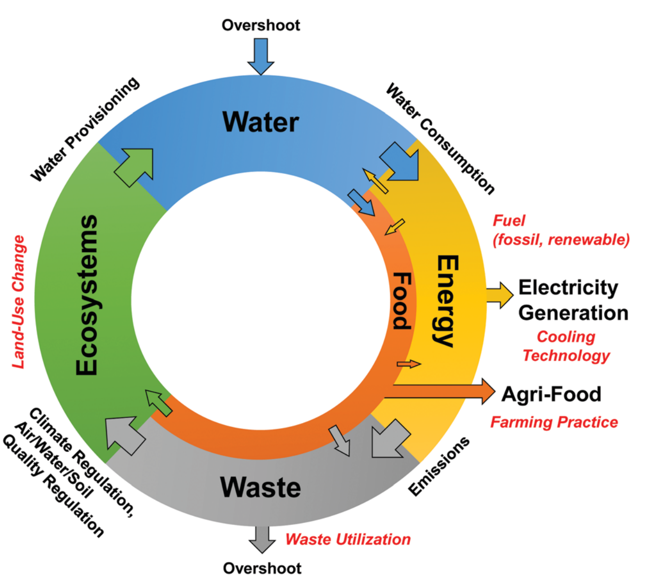


Fig. 1 Framework for techno-ecologically synergistic food–energy–water (TES-FEW) nexus. Orange, yellow, blue, green, and gray-colored arrows represent food, energy, water, ecosystem, and waste flows, respectively. Technological and agro-ecological options that affect those flows are shown in red italics.

Food systems also influence ecosystem flows such as the soil carbon sequestration service. The TES-FEW nexus framework shows greater interactions between FEW flows than the original framework by accounting for the interactions of FEW systems with ecosystems.

Changes in FEW systems and ecosystems, shown in red italics in Fig. 1, will affect the magnitude and intensity of each flow. Various potential strategies can be considered for each FEW nexus component to improve the economic feasibility and ecological viability of FEW systems. Fig. 2 summarizes such alternatives that are considered in this work. With respect to energy systems, different fuel options, power generation technologies, and cooling technologies can be considered as alternatives for more sustainable power generation. For instance, coal-fired steam turbine (CST) power plants are replaced by natural gas-fired combined cycle (NGCC) plants. Renewable energy sources such as solar and wind power are emerging as solutions for sustainable power generation. Also, cooling technologies for power plants have been converted to water-efficient technologies (recirculating and dry cooling). Moreover, to mitigate CO_2 emissions, industries are striving to develop and implement CO_2 conversion technologies which will be likely to require substantial energy and water. These technological alternatives can be characterized by the clean power plant (CPP) strategy, which aims to contribute to sustainable energy systems by reducing impacts while meeting the societal demand for affordable electric power.

In addition to technological alternatives, agro-ecological alternatives can be considered for sustainable FEW systems. Farmers could consider different farming practices, such as converting from conventional tillage to no-till. Also, land-use change options could be considered as ecological alternatives since ecosystem flows are sensitive to land-use and land-cover. For example, barren land areas can be reforested to enhance ecosystem services such as climate and air quality regulation. Wetlands can be constructed on the barren areas to improve ecosystem services, such as nutrient retention and freshwater provisioning.

Alternatives in Fig. 2 will affect multiple flows and their interactions at the TES-FEW nexus. To discover solutions for sustainable FEW systems, a systematic modeling approach is needed since we need to capture numerous interactions among multiple activities[20,21] from the superstructure in Fig. 2. In this work, we perform a case study to investigate the sustainability of various FEW-related activities, which include fuel mining, thermoelectric and renewable power generation, CO_2 capture and conversion, farming, and ecological land use in the MRW. The upstream life cycle stages of activities in the MRW are taken into consideration in this study to reduce the chance of burden shifting. Extensive data need to be collected from numerous databases for such work. They are shown in Section S1 (ESI†). Monetary and environmental data for each of the activities and alternatives vary with regions. In this study, regional data for the MRW are used when available. For instance, facility-level

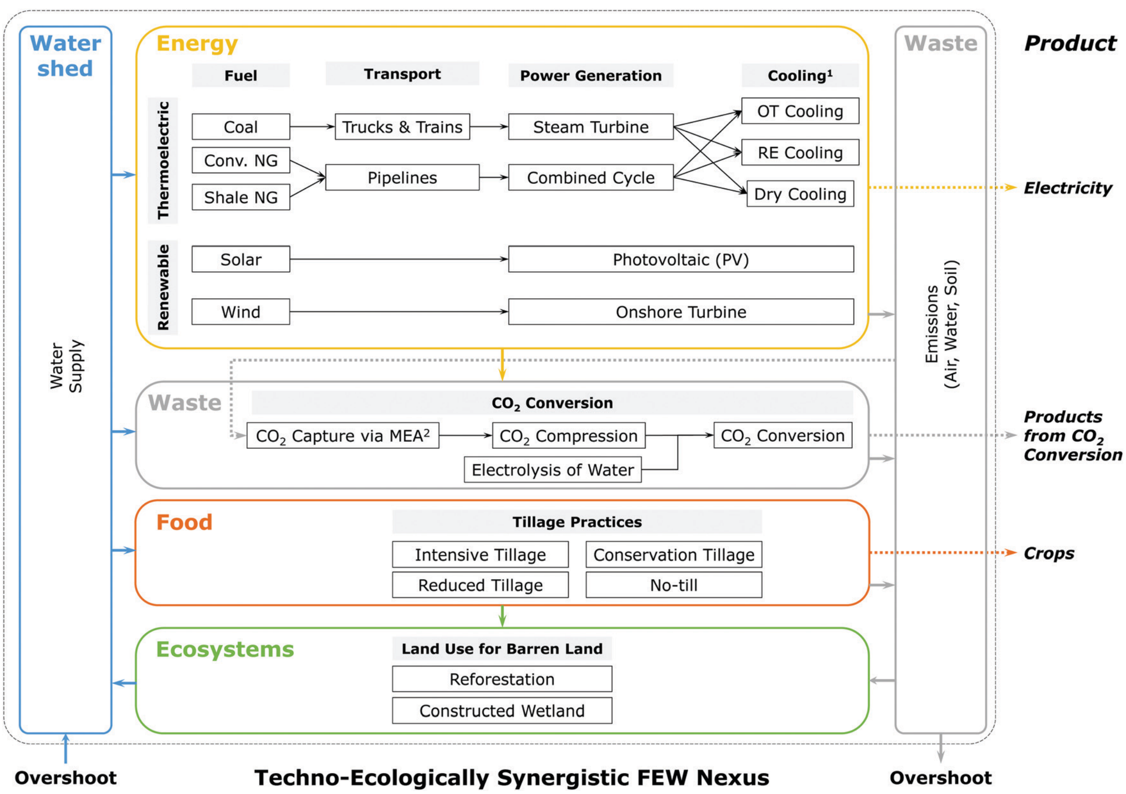


Fig. 2 Alternatives for sustainable FEW systems in this work and their interactions at the TES-FEW nexus. Various FEW-related activities in a watershed and their upstream life cycle stages are taken into account in this study. [1]OT: once-through, RE: recirculating. [2]MEA: monoethanolamine.

greenhouse gas (GHG) emission and resource use data for thermoelectric power generation in the MRW are available from the Emissions and Generation Resource Integrated Database (eGRID)[22] and Form EIA-923,[23] respectively. Also, the Soil and Water Assessment Tool (SWAT) model[24] and i-Tree models[25,26] are used to estimate various water and ecosystem flows in the MRW, respectively. Some regional data such as cost are hard to obtain. In such a case, national data from online sources and literature reports are used. For example, data from the Greenhouse gases, Regulated Emissions, and Energy use in Technologies (GREET)[27] model are employed to calculate GHG emissions and water consumption for mining and renewable power generation activities.

The case study is conducted as follows. First, we investigate the sustainability characteristics of FEW systems in the MRW for the year 2014 (defined as the base case) by quantifying the environmental impacts of FEW-related activities and the benefits of ecosystems. This year is selected for the case study since some data are not available for the years after 2014 at this point. In this work, we consider the time period to be one year. Ecological overshoot is identified by calculating techno-ecological synergy (TES) metrics (V_k) for the k-th ecosystem service.[6] Details about these metrics are provided in Section 2.2.3.

Then, we explore alternative management strategies shown in Fig. 2, while identifying the interactions of FEW systems with ecosystems. Two domains of alternative strategies are considered: technological and agro-ecological. The former corresponds to techno-centric strategies, while the latter represents techno-ecologically synergistic strategies. For various alternatives, we consider each alternative to be fully employed in the MRW (*e.g.*, complete replacement of coal with shale gas for power generation). That is, activities in the MRW are homogeneous within the watershed for every alternative case. Also, sensitivity analysis is performed for uncertain data in emerging technologies, such as renewable power generation. The effect of each alternative on economic, social, and ecological aspects is quantified by indicators of profit, social cost, and ecological overshoot. More details on the indicators are in Sections 2.2.3 and 2.3.

Lastly, we explore potential solutions that could improve the sustainability of FEW systems while meeting multiple stakeholders' needs. Here, we do not solve mathematical optimization problems but rather investigate solutions by combining various strategies from multiple domains in Fig. 2 to obtain insights on how each alternative affects the sustainability of FEW systems. In Section S2 (ESI†), we describe the characteristics of existing activities that include mining, thermoelectric power generation, and farming in the MRW. In the following, we describe renewable power generation, CO_2 conversion technologies, and ecosystem services that we consider in this work.

2.2 Technological and ecological alternatives for FEW systems

2.2.1 Renewable power generation. To reduce the impacts of utilizing fossil fuels, renewable energy sources such as solar and wind power are considered as alternative power generation technologies. In 2018, 1.5% and 6.5% of electricity were generated from solar and wind resources in the U.S., respectively,[28] and these shares are expected to increase. Renewable technologies require less water and have fewer emissions than thermoelectric power generation technologies. For solar power generation, concentrated solar power (CSP) technology needs a similar amount of water as thermoelectric technologies to generate electricity since the CSP technology requires cooling of solar panels and steam turbines. In 2018, CSP accounted for only 6% of solar power generation in the U.S.[23] The remaining 94% utilize photovoltaic (PV) technology. Unlike the CSP technology, PV technology does not require much water for generating electricity: it needs only a small amount of water for cleaning the surface of solar panels.[29] Wind power generation technology does not need any water as well. Moreover, solar and wind power generation technologies do not have direct air and water emissions.

In this work, we assume solar PV and wind power generation technologies can be employed in the MRW. The power density of solar PV energy is known to be much higher than that of wind energy.[30,31] Based on modern solar PV panels and wind turbines,[32,33] we consider that 15–20% and 35–45% of solar and wind energy can be converted into electricity. Each solar panel and wind turbine needs to be spaced from its neighbors to avoid interference from them (*i.e.*, shade caused by the neighboring panels and aerodynamic losses between turbines). In this study, solar panels are assumed to occupy 70% of the solar farm area.[34] Spacing between wind turbines is typically 5–10 rotor diameters,[35,36] which means that approximately 2–6% of the wind farm area is occupied by the turbines. In this work, we assume 4% of the wind farm area is occupied by the turbines. Considering regional solar and wind energy potentials in the MRW,[37] we estimate that 5.78–7.71 m^2 and 127–163 m^2 of land area are required for solar and wind power generation to generate 1.0 MW h per year of electricity, respectively.[37] In addition, since renewable technologies replace conventional thermoelectric technologies, we consider that displacement credits can be given to renewable technologies. That is, upstream life cycle emissions associated with the thermoelectric generation technologies can be avoided by employing renewable technologies.

Although renewable generation technologies have many strengths in terms of environmental impacts compared to thermoelectric technologies, they also have some shortcomings. One of the biggest challenges is the intermittency of power sources. The available amount of solar and wind power depends on location and time with uncertainties. Therefore, technologies need to be employed with energy storage systems. In this work, however, we do not consider those systems due to a lack of data. Also, additional impacts and costs will be associated with decommissioning and recycling solar PV panels and wind turbine blades, given that the average lifetime of solar PV panels and wind turbine blades is 20–25 years.[38,39] Due to the large uncertainty in their impacts and costs, the end-of-life phase of renewable power generation is excluded from the scope of this study. In addition, renewable power plants need to employ more minerals such as copper, zinc, and silicon than fossil power plants.[40] Direct-drive wind turbines require the use of rare-earth elements such as neodymium for permanent magnet generators.[41]

Generating wind power also has small climatic impacts due to the redistribution of heat within the atmosphere by turbines.[42] Moreover, since solar and wind power technologies require a large land area, these renewable generation technologies may compete with other activities for the limited land area. Farming activities for food production and ecological activities (*e.g.*, forests and wetlands) for providing ecosystem services require a huge land area as well.

For renewable generation technologies to be economically feasible, they need to be cheaper than thermoelectric generation technologies. When we do not consider any monetary credits for utilizing renewable power sources, the levelized costs of electricity (LCOE) for newly entering conventional NGCC, solar PV, and onshore wind power plants in 2023 are estimated to be \$42.8, 48.8, and 42.8 per MW h, respectively.[43] If federal tax credits are considered for renewable power sources, the LCOE for solar PV and onshore wind power plants are reported to be \$37.6 and 36.6 per MW h, respectively, which are cheaper than the conventional NGCC plants. Therefore, renewable power generation technologies can be economically feasible if tax incentives are considered. In this work, we employ the LCOE without tax credits for renewable technologies. Therefore, our results represent a worst-case scenario for these technologies.

2.2.2 CO_2 conversion technologies. To reduce environmental impacts from human activities, waste materials can be utilized by recycling them or converting them into other valuable products. In this paper, we focus on CO_2 capture and conversion strategies. To mitigate global warming, various CO_2 conversion pathways and technologies have been studied.[44,45] As one of the pathways, CO_2 can be captured from stationary point sources such as fossil power plants through pre- and post-combustion technologies or from the air by direct air capture technology.[46] The captured CO_2 can be converted to various hydrocarbon products such as methane, synthetic gas, formic acid, urea, and methanol, which can be used for many industrial uses.

Fig. 3 shows CO_2 capture and conversion processes. We assume that CO_2 emissions from fossil power plants in the MRW are captured through monoethanolamine (MEA) absorption, compressed, and converted to methane, syngas, or formic acid. MEA-based carbon capture is considered in this work since it is one of the most mature capture technologies, and its life cycle inventory (LCI) data is available from existing databases.[47] Hydrogen for hydrocarbon products is assumed to be provided from water through the electrolysis process. Also, we assume that newly-developed CO_2-converted methane, syngas, and formic acid products in the MRW displace NG, syngas, and formic acid that are produced using conventional technologies, respectively.

Carbon capture and conversion technologies tend to be energy-intensive. The capture process using 15–20% of MEA solution requires 0.4 kW h for 1 kg of CO_2.[47] As shown in Fig. 3, the captured CO_2 needs to be compressed to a high pressure, which requires the use of electricity as well. Also, many CO_2 conversion processes are highly energy-intensive. For example, CO_2 can be converted to methane through the Sabatier reaction:

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O \quad \left(\Delta_R H^{\circ}_{298} = -165\ \text{kJ mol}^{-1}\right) \tag{1}$$

If we consider that hydrogen is produced from water by electrolysis, this process requires energy as follows:

$$H_2O \rightarrow H_2 + 0.5O_2 \quad \left(\Delta_R H^{\circ}_{298} = 286\ \text{kJ mol}^{-1}\right) \tag{2}$$

As a result, the overall conversion process from the captured CO_2 to methane is described by,

$$2H_2O + CO_2 \rightarrow CH_4 + 2O_2 \quad \left(\Delta_R H^{\circ}_{298} = 979\ \text{kJ mol}^{-1}\right) \tag{3}$$

CO_2 can also be used to produce carbon monoxide through the reverse water–gas shift reaction and formic acid through the hydrogenation of CO_2 as shown in the following reactions,

$$CO_2 + H_2 \rightarrow CO + H_2O \quad \left(\Delta_R H^{\circ}_{298} = 41\ \text{kJ mol}^{-1}\right) \tag{4}$$

$$CO_2 + H_2 \rightarrow HCOOH \quad \left(\Delta_R H^{\circ}_{298} = -31.5\ \text{kJ mol}^{-1}\right) \tag{5}$$

CO_2-converted carbon monoxide from eqn (4) can be combined with hydrogen from eqn (2) to produce syngas.

Since these conversion processes need to utilize the electrolysis of water shown in eqn (2), the conversion processes are not only energy-intensive but also water-intensive. Moreover, the carbon capture process requires additional water for cooling.[48] If electricity for the CO_2 capture and conversion processes is provided from conventional thermoelectric power plants, total energy and water consumption including the upstream processes will be significantly large. Therefore, renewable power generation technologies that have smaller emissions and resource consumption need to be considered for providing electricity to the conversion processes.[49]

The CO_2 capture and conversion processes are also economically expensive. In this work, we employ data from the existing studies.[50–52] For instance, Pérez-Fortes *et al.* (2016) estimated that the production cost for CO_2-converted formic acid is more than 3 times the cost of conventional formic acid through the methyl

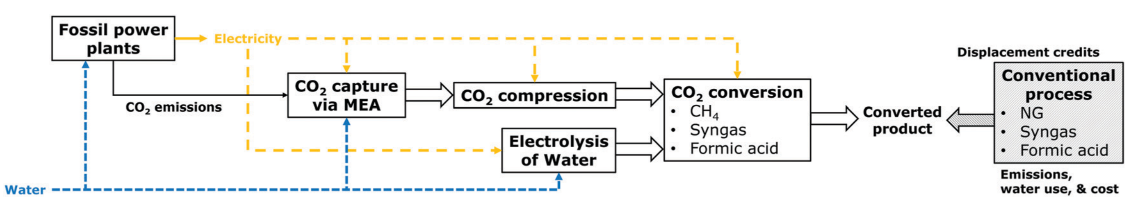


Fig. 3 Energy- and water-intensive CO_2 capture and conversion processes. The converted products displace the products from conventional processes.

formate hydrolysis process, primarily because of the large resource and utility consumption for the conversion processes.[52]

We assume that the CO_2-converted products will replace the products from conventional processes. For example, CO_2-converted methane is assumed to displace NG from the fossil fuel extraction process. CO_2-converted CO can be used to make synthesis gas by combining with hydrogen. Syngas is produced conventionally through the gasification of coal or by steam reforming of NG.[53] In this paper, steam reforming of NG is identified as the conventional syngas production process since the production of NG has increased significantly due to the shale gas boom. As shown in Fig. 3, environmental impacts and costs for the conventional processes can be avoided and considered as displacement credits to the CO_2 conversion technologies.

In this study, we consider the market demand for CO_2-converted products given that the worldwide potential market of CO_2 utilization for chemical conversion was estimated to be less than 10^{12} kgC per year based on the global production of all hydrocarbon chemicals.[44] Also, the global liquid fuel production was estimated to be 2.1×10^{12} kgC per year.[44] Given that global CO_2 emissions from the combustion of fossil fuels in 2016 were 8.8×10^{12} kgC,[54] therefore, it is important to consider the market demand for CO_2-converted products. With respect to formic acid, for example, its global production capacity in 2013 was 6.97×10^8 kg.[52] Stoichiometrically, this corresponds to only 1.82×10^8 kgC per year if formic acid is produced from the hydrogenation of CO_2. In this study, therefore, we assume 400 000 t per year of CO_2 (= 1.09×10^8 kgC per year) are converted to hydrocarbons. Future cost reduction of conversion technologies could expand their potential uses and lead to an increase in market size for the CO_2 conversion.

Unlike other activities described in this section, CO_2 conversion technologies have not been fully commercialized yet. Therefore, it is challenging to obtain reliable data for the conversion processes. Experimental data are available from numerous sources. However, they are based on different process configurations such as different catalyst use, conversion ratio, temperature, and pressure. For instance, while one study was performed by employing 120 bar of CO_2 pressure for converting CO_2 to formic acid,[55] others employed 30 bar.[56–58] Due to these difficulties, we assume 30 bar of CO_2 pressure for stoichiometric CO_2 conversion reactions for the simplicity of analysis in this work.

2.2.3 Ecosystem services. Ecosystem services are the basis for all human activities.[59] To avoid ecological overshoot, the supply of ecosystem services must be considered because environmental interventions from human activities could, and often do exceed nature's capacity. The framework of Techno-Ecological Synergy (TES) has been developed to account for the supply of ecosystem services in the modeling work.[6] This framework calculates TES sustainability indices (V_k) for each ecosystem flow (k) by,

$$V_k = \frac{S_k - D_k}{D_k}, \quad (6)$$

where $V_k \geq -1$. Variables, S_k and D_k represent the supply and demand, respectively, for the k-th ecosystem service. In terms of CO_2 flow, for instance, S_{CO_2} and D_{CO_2} correspond to the carbon sequestration service provided by various ecosystems, and CO_2 emissions from human activities. V_k must be non-negative to avoid ecological overshoot and claim absolute sustainability for that ecosystem service.

In calculating V_k metrics, selection of the analysis boundary is important since the scale of beneficiaries (serviceshed) for each ecosystem service depends on its characteristics.[17] For example, the serviceshed for climate regulation is global, while that for water provisioning is the watershed. Also, if D_k represents interventions from a specific activity, S_k needs to be allocated to that activity because ecosystem services are beneficial to every activity in the serviceshed.[60] For the modeling work in this study where multiple activities are considered, D_k can be the intervention from every activity in a region. In such a case, S_k needs to represent the whole supply in the region and V_k can be calculated for all activities in the region.

In this paper, we focus on three types of ecosystem services: freshwater provisioning, climate regulation, and nutrient retention. The water provisioning service considers various factors in the water cycle such as precipitation, evapotranspiration, infiltration, and surface/subsurface runoff. Several tools are available to estimate the water provisioning service. Table S1 (ESI†) summarizes the tools employed in this work. For example, the SWAT model calculates water yield to streamflow in a watershed.[24] Water Global Assessment and Prognosis (WaterGAP) hydrology model has been developed to calculate the amount of available water on a global scale while accounting for factors in the water cycle.[61] Available Water Remaining (AWARE) model, which is based on the WaterGAP model, can also be used to calculate the amount of available water.[62] In this work, we used the SWAT model to simulate the effects of farming practices on water yield, nutrient runoff, and agricultural production.[63]

Ecosystem flows are sensitive to land-use and land-cover. For the water provisioning service, wetlands improve the supply of freshwater by removing water contaminants and excessive nutrients from wastewater. i-Tree Hydro can simulate the effect of land-use change on the water provisioning service.[25] Wetlands provide the nutrient retention service as well. Kadlec (2008, 2016) investigated how much nitrogen and phosphorus could be removed by constructed wetlands.[64,65] With respect to climate regulation, wetlands sequester CO_2 but release CH_4 whose contribution to global warming is 25 times greater than CO_2 emissions. Whiting and Chanton (2001) studied the impacts of wetlands on global warming.[66] They identified that the overall effects of wetlands on climate change vary with geographic location and time horizon. In this study, we ignore these effects due to a lack of region-specific data.

Forests affect various ecosystem services as well. Forest ecosystems provide climate regulation, air quality regulation, and biomass provisioning services. Regional data can be obtained from various i-Tree tools such as i-Tree County Benefits and i-Tree Landscape.[26] Reforestation strategies such as land-use change from barren lands to forests could enhance those ecosystem services. However, reforestation could decrease water provisioning service, as modeled by i-Tree Hydro.[25] Filoso *et al.* (2017) reviewed the impacts of reforestation on water yield.[67]

They concluded that water yield is reduced in the short term and recovered in the long term due to improved soil infiltration. In this work, we employ i-Tree Hydro to examine the effects of reforestation on water provisioning.

Ecological strategies to improve the supply of ecosystem services could be economically low cost solutions. For example, the USDA's report estimated tree establishment costs for Ohio to be around \$500 per ha.[68] The capital costs for constructed wetlands were estimated to be \$69 000 per ha for large wetlands and \$132 000 per ha for small wetlands.[65] Also, those ecological strategies do not require many operation and maintenance (O&M) expenses. Non-commercial reforestation only requires \$10 per ha per year of O&M cost,[69] and large and small constructed wetlands require \$3620 per ha per year and \$770 per ha per year of O&M costs, respectively.[65] In this work, we employ the median capital and O&M costs for constructed wetlands.

The supply of ecosystem services could be monetized to obtain aggregate indicators that indicate the extent to which relevant ecosystems contribute to society. The impact of economic activities on ecosystems could then be quantified as the external cost or public cost, since it is incurred by society and is usually excluded in conventional markets. Such monetary valuation of ecosystem services varies with their location since each region has a different population, weather, land-use and land-cover, and tree species. Collecting such region-specific data for the valuation of ecosystem services could be time-consuming and expensive. Therefore, in this work, we use the benefit transfer method to monetize regional ecosystem services.[70,71] According to this method, the monetary value (*e.g.*, \$ per ha) of the benefits of ecosystem services in a study region can be estimated from the value that has been investigated already for another region that has similar regional characteristics as the study region. In this study, the value for the benefits of ecosystem services is obtained from the Environmental Valuation Reference Inventory.[72]

2.3 Sustainability indicators

In this section, we describe how various sustainability indicators are calculated in this work. Note that each indicator is defined such that a larger value indicates improvement and is preferred. Multiple objectives need to be considered to perform the FEW nexus study to account for various interactions between FEW flows and ecosystem flows. We consider seven indicators: three TES indices (V_{CO_2}, V_N, and V_{water}), marginal net electricity generation, marginal corn production, marginal profits, and marginal external benefits. For the comparison, 8.4×10^4 TJ per year of annual electricity generation is fixed regardless of alternative options adopted. The marginal values are based on comparison with the base case. Net electricity generation corresponds to the aggregated electricity generation minus aggregated consumption by activities in the MRW. Thus, the marginal net electricity generation (MNEG) is calculated as follows,

$$\mathrm{MNEG} = \left(\sum_i^n \mathrm{EG}_i - \mathrm{EC}\right) - \left(\sum_i^n \mathrm{EG}_{\mathrm{base},i} - \mathrm{EC}_{\mathrm{base}}\right), \quad (7)$$

where $i = 1,2,\ldots,n$ correspond to power plants. EG_i and EC represent electricity generation (the output of the generator) from each power plant i and aggregated electricity consumption in the MRW, respectively. EC includes parasitic loads to generate electricity from the power plants. A subscript base means base case values. Similarly, the marginal corn production (MCP) is calculated as follows,

$$\mathrm{MCP} = \sum_{i'}^{n'} \mathrm{CP}_{i'} - \sum_{i'}^{n'} \mathrm{CP}_{\mathrm{base},i'}, \quad (8)$$

where $i' = 1,2,\ldots,n'$ correspond to farms. $\mathrm{CP}_{i'}$ is the amount of corn production from each farm i'.

With respect to two monetary objectives, the marginal profits refer to the change in profits for plant operators by employing alternative options. The marginal profits (MP) are calculated as,

$$\mathrm{MP} = \sum_j^m \left(p_j \times \mathrm{Prod}_j - \mathrm{Cost}_j\right) - \sum_j^m \left(p_j \times \mathrm{Prod}_{\mathrm{base},j} - \mathrm{Cost}_{\mathrm{base},j}\right), \quad (9)$$

where $j = 1,2,\ldots,m$ correspond to products, and p_j represents unit price of product j. The market price of products is assumed to be fixed over alternative options in this study. Prod_j and Cost_j correspond to the physical amount of production for products j and the monetary cost for the production, respectively. In case of electricity, $\mathrm{Prod}_{\mathrm{elec}}$ is equal to $\left(\sum_i^n \mathrm{EG}_i - \mathrm{EC}\right)$ in eqn (7). On the other hand, the marginal external benefits mean the change in external benefits to society from reducing environmental damages. The marginal external benefits (MEB) are calculated by eqn (10):

$$\mathrm{MEB} = \sum_k^l \{c_k \times (S_k - D_k)\} - \sum_k^l \{c_k \times (S_{\mathrm{base},k} - D_{\mathrm{base},k})\}, \quad (10)$$

where $k = 1,2,\ldots,l$ correspond to ecosystem flows. Variable c_k represents the unit external cost borne by society to absorb environmental damages. This cost is obtained in this work by using the benefit transfer method.[70,71] If the external costs and benefits are internalized in the market, the marginal change in total profits is equal to MP + MEB.

3 Results and discussion

3.1 The study region

Five thermoelectric power plants (two CST and three NGCC) were operating in the MRW in 2014. There were no renewable power plants and CO_2 conversion facilities in this region. The primary crops produced in the MRW were mostly corn and some soybean with the implementation of no-till (57%) and tillage practices (43%). Also, 0.32% of land-use in the MRW was barren land. This status is defined as the base case. Additional details about activities in the MRW for the base case are available in Section S3 (ESI†).

Table 1 summarizes multiple indicators (V_k metrics, productivity, and monetary) for the base case and cases where each alternative is

Table 1 Summary of the results for various alternatives investigated in this work

				V_k metrics[a]			Marginal values[b]			
Domain	Nexus elements	Alternative categories	Alternatives	CO_2	N	Water	Net E. gene. (10^3 TJ per year)	Corn prod. (10^3 t per year)	Profits (10^6 \$ per year)	Ext. benefits[c] (10^6 \$ per year)
Base case				−0.914	−0.993	49.8	0	0	0	0
Technological (techno-centric strategies)	Energy	Fuel (thermoelectric)	CST w.RE	−0.937	−0.993	41.3	−3.78	0	−443	−222
			Conv. NGCC w.RE	−0.869	−0.992	58.5	2.81	0	−437	202
			Shale NGCC w.RE†	−0.868	−0.992	56.0	2.81	0	418	202
	Water	Cooling[d]	Shale NGCC w.OT	−0.868	−0.992	79.9	3.32	0	481	203
			Shale NGCC w.RE†	−0.868	−0.992	56.0	2.81	0	418	202
			Shale NGCC w.Dry	−0.870	−0.992	166.0	0.61	0	206	198
	Energy	Fuel (renewable)[e]	Solar PV adopted	−0.857	−0.992	60.0	3.05	0	417	233
			Wind adopted	−0.868	−0.992	56.1	2.82	0	419	203
	Waste	CO_2 conversion[f]	Conv. to methane	−0.913	−0.993	43.6	−9.64	0	−1078	4
			Conv. to syngas	−0.911	−0.993	44.0	−8.57	0	−1053	20
			Conv. to formic acid	−0.909	−0.993	51.8	−2.75	0	−600	31
	Energy-water-waste	Technological solution (Shale NGCC w.RE, solar PV adopted, and CO_2 conv. to formic acid)		−0.843	−0.992	63.0	0.31	0	−196	264
Agro-ecological (TES[g] strategies 1)	Food	Tillage practices	No-till	−0.912	−0.993	49.8	0	−0.25	0.90	1.14
			Conserv. till	−0.914	−0.993	49.7	0	0.12	−1.22	−0.57
			Reduc. till	−0.917	−0.993	49.7	0	0.59	−1.14	−2.39
			Intens. till	−0.918	−0.993	49.6	0	0.83	−1.10	−3.49
	Ecosystem	Land use	Reforestation	−0.913	−0.991	49.7	0	0	−0.02	2.90
			Wetland	−0.914	−0.976	49.8	0	0	−4.15	0.27
	Food–ecosystem	Agro-ecological solution (no-till and wetland)		−0.912	−0.976	49.9	0	−0.25	−3.26	1.41
Synergistic (TES[g] strategies 2)	Food–energy–water-ecosystem	Synergistic solution (technological + agro-ecological solutions and agrivoltaic systems[h])		1.094	−0.974	222.1	2.57	1.07	−213.84	563

[a] V_k metrics represent absolute sustainability with respect to k-th flow. [b] Marginal values are based on comparison with the base case. [c] External benefits correspond to the monetized benefits of ecosystem services to society. [d] OT, RE, and dry indicate once-through, recirculating, and dry cooling technologies, respectively. [e] In addition to the shale NGCC plants with recirculating systems (†), renewable power plants are installed on the barren lands while displacing the shale NGCC plants. [f] The amount of converted-CO_2 is 400 000 t per year. [g] TES stands for techno-ecologically synergistic. [h] 60.9% of farmlands adopt agrivoltaic systems.

employed. External benefits correspond to the monetized benefits of ecosystem services to society. Additional in-depth discussion of alternatives is available in Sections S4 and S5 (ESI†). Also, detailed data for figures and tables are available in Supplementary Information 2 (ESI†).

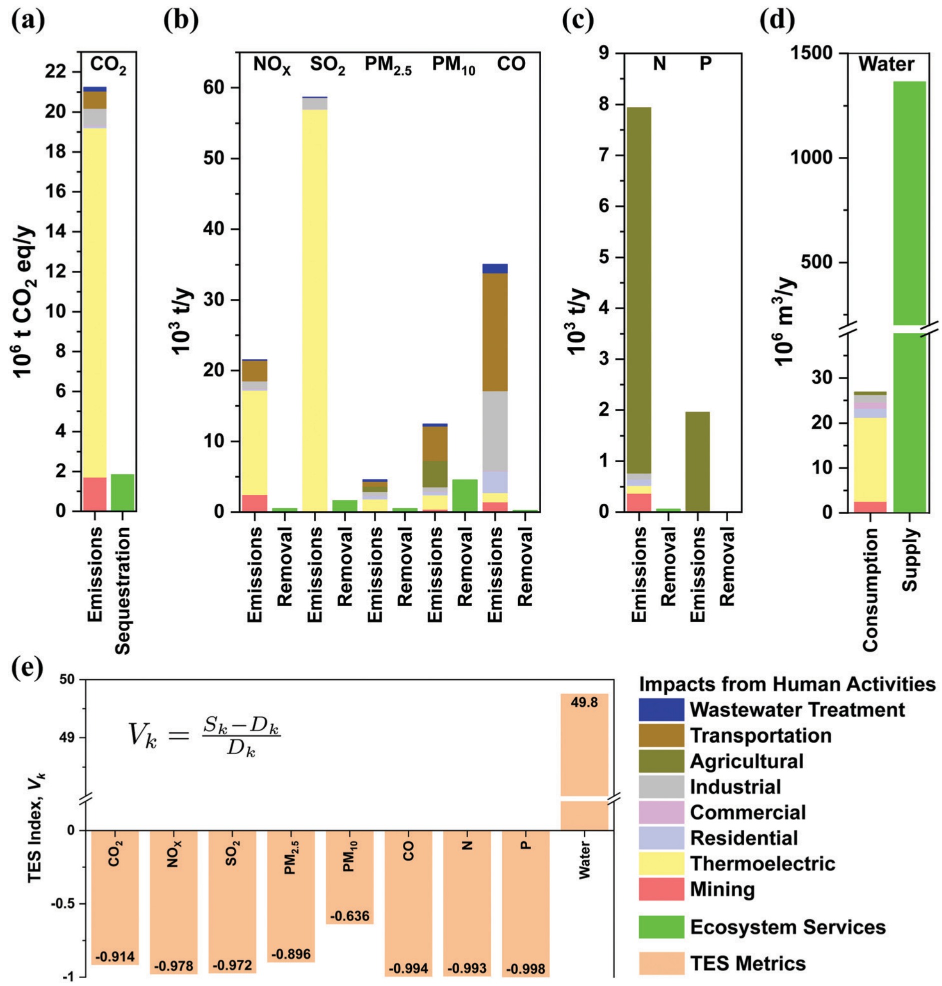
3.2 Base case results

Fig. 4 presents the environmental impacts of various FEW-related activities (*i.e.*, the demand for ecosystem services: D_k) and the supply of ecosystem services (S_k). Also, the TES metrics (V_k) are calculated for each flow (k) by $V_k = (S_k - D_k)/D_k$. The background concentrations of the emissions (*e.g.*, nutrient runoff upstream to the MRW) are not included. Every V_k index except for V_{water} is close to negative one (−1). This indicates unsustainable conditions of activities in the MRW in terms of ecosystem services flows. Positive V_{water} represents that this region does not suffer from water shortage. Therefore, the MRW could potentially be managed by employing water-intensive alternatives for sustaining the productivity of FEW systems. Alternatives need to be considered for thermoelectric and agricultural activities since most interventions are primarily attributed to those activities. Additional discussion on thermoelectric power plants in the MRW is available in Section S3 (ESI†). Also, land-use change options can be considered to enhance the supply of ecosystem services. In the following section, we explore various solutions for the FEW nexus in the MRW.

3.3 Techno-centric strategy

Thermoelectric power generation is a huge contributor to most of the environmental impacts, as is apparent from Fig. 4(a), (b) and (d). Technological strategies considered in this study include the replacement of coal by NG, water-efficient cooling, renewable power sources, and CO_2 capture and conversion to hydrocarbons. Among various environmental indicators, we focus on CO_2 (as air emissions), N (as water emissions), and water consumption indicators.

As shown in Table 1, among fossil fuels, shale NGCC is not only better for environmental sustainability ($V_{CO_2} = -0.868$) but is also economically profitable. Positive marginal profits (\$418 million per year) and external benefits (\$202 million per year) are expected by employing shale gas for power generation. Comparison between conventional NG and shale NG options shows no significant differences in environmental indicators because mining activities account for relatively small portions of the overall environmental interventions as shown in Fig. 4. Extracting shale gas by hydraulic fracturing has been known to consume more water[73] and release



$$V_k = \frac{S_k - D_k}{D_k}$$

Fig. 4 Base case demand and supply of ecosystem services in the MRW. (a) Climate regulation (greenhouse gases), (b) air pollutant, (c) water nutrient emissions, and (d) water consumption. For all ecosystem services except water provisioning, demand exceeds exceed the supply. (e) TES sustainability metrics for each ecosystem service. Activities in the MRW respect nature's capacity only for water consumption.

more water pollutants.[74,75] The study on the NG extraction in the Appalachia region, where the MRW is also located, reported that nitrogen emissions to water from shale gas extraction are approximately 300 times larger than those from conventional NG extraction.[76] However, the results in this study show that from the perspective of watershed-scale sustainability, the increased interventions for the shale gas option are relatively insignificant. Rather, exploiting shale gas makes sense because it is more cost-effective than conventional NG.[77–79] The cost of shale gas production, however, may increase to maintain its production as shale wells are depleted.[79,80]

Also, dry cooling is extremely effective for improving the water sustainability indicator (V_{water} = 166.0). However, for a region such as the MRW, recirculating cooling could be preferred since dry cooling is very expensive ($212 million per year less profitable) compared to recirculating cooling, and water is not scarce in this watershed.

In the CPP strategy, increasing the use of renewable power sources is one of the primary alternatives for reducing the environmental impact of power generation. If we assume that the barren land area (1.30×10^7 m^2) in the MRW can be utilized for renewable power generation, 6.1–8.1 and 0.3–0.4 thousand TJ per year of electricity can be generated from solar and wind power sources, respectively.[37] These correspond to approximately 7.2–9.6% and 0.3–0.4% of total electricity generated from the fossil power plants in the MRW, respectively. The sensitivity analysis results in Table S2 (ESI†) show that the results are robust. Therefore, only the best case results (20% of PV module efficiency and 45% of wind turbine efficiency) are shown and discussed in this section.

Both solar PV and wind power plants have similar intervention intensities for metrics, such as kg CO_2 emissions per MJ of electricity generation, which are very small compared to fossil power plants. However, since solar power has a higher energy potential per area than wind power, larger (better) environmental metrics, V_{CO2} and V_{water}, can be obtained with the solar power option. With respect to monetary aspects, the solar PV option is less profitable than the wind and shale NGCC options since it has a higher LCOE.[43] However, if we consider the environmental external benefits, the monetary benefits of avoiding environmental damages for the solar PV option outweigh its lower profits. This implies that internalizing external benefits could change decisions from the monetary point of view.

CO_2 conversion technologies are promising alternatives to mitigate global warming by converting CO_2 into valuable hydrocarbon products. In this study, we assume that CO_2 emissions from fossil power plants in the MRW are captured by absorption in MEA followed by compression and conversion to methane, syngas, or formic acid, as shown in Fig. 3. Hydrogen for hydrocarbon products is assumed to be provided by the electrolysis of water. In this work, 400 000 t per year of CO_2 conversion is assumed for the three conversion options. Also, we assume that newly-developed CO_2-converted methane, syngas, and formic acid products in the MRW displace NG, syngas, and formic acid that are produced using conventional technologies, respectively.

CO_2 emissions, water consumption, electricity consumption, and production costs for each conversion option are shown in Table 2. Overall, the formic acid option shows the most promising results among the conversion options. The V_{CO_2} indicator for this option is the highest due to its higher CO_2 credits from displacing the conventional formic acid manufacturing process (methyl formate hydrolysis). All conversion options are water-intensive processes not only because the CO_2 capture process requires a substantial amount of water[48] but also because water is used to provide hydrogen to hydrocarbons. However, due to the large displacement credits from the conventional process, the formic acid option exhibits an increase in the V_{water} indicator. Also, the formic acid option is the least energy-intensive CO_2 conversion option because of its lower energy requirement for the CO_2 conversion process compared to other options.[81] Accordingly, the formic acid option is more lucrative than the other conversion options.

The high energy requirement and cost for CO_2 conversion processes are among the key barriers to the deployment of these technologies. However, negative marginal profits and net electricity generation of the conversion options can be minimized by employing CO_2 conversion with other technological alternatives. In this study, when we employ shale NGCC power plants with recirculating systems and adopt solar PV power plants in the available lands, the marginal profits are positive ($417 million per year) because this alternative case is more economically beneficial than the base case, which has two coal power plants without any renewable power plant. The alternative case becomes less profitable when we employ CO_2 conversion options as shown in Fig. S5 (ESI†). For the formic acid option, the marginal profits become negative when 300 000 t per year of CO_2 are converted. However, if we internalize external benefits from mitigating environmental damages, CO_2 conversion technologies can be more economically competitive. The external benefits are slightly increased as more CO_2 is converted, and marginal change in total profits (the sum of profits and external benefits) can be positive for 400 000 t per year of CO_2 conversion to formic acid. This implies that the internalization of the external benefits could promote the use of advanced technologies that mitigate environmental damages but are economically expensive. Such internalization will require policies such as carbon taxes or cap and trade.

The CPP strategy can be an effective solution for improving the V_{CO_2} indicator and mitigating climate change. In this study, the technological solution includes the replacement of coal by shale gas for generating electricity, recirculating cooling, the adoption of solar power plants (with 20% PV module efficiency) in the available lands, and 400 000 t per year of CO_2 conversion to formic acid. As shown in Table 1 and Fig. 5, V_{CO_2} for the solution is −0.843 which is better than −0.914 for the base case. The solution can also improve the V_{water} indicator significantly (from 49.8 to 63.0). V_N indicator, however, does not change much for technological alternatives. This is because N runoff is mainly due to agricultural activity, as shown in Fig. 4. The solution shows trade-offs between environmental

Table 2 Detailed results for CO_2 conversion options about CO_2 emissions, water consumption, electricity consumption, and production costs

	CO_2 emissions [10^3 t per year]	Water consumption [10^6 m^3 per year]	Electricity consumption [10^3 TJ per year]	Production costs [10^9 $ per year]
Methane				
CO_2 capture	317.45	3.47	0.61	0.02
CO_2 conversion[a]	−400.00	0.33	9.06	0.77
Displacement credits[b]	−66.53	−0.08	−0.03	−0.02
Total	−149.08	3.72	9.64	0.77
Syngas				
CO_2 capture	317.45	3.47	0.61	0.02
CO_2 conversion[a]	−400.00	0.33	8.34	0.83
Displacement credits[b]	−664.75	−0.33	−0.38	−0.07
Total	−747.29	3.46	8.57	0.78
Formic acid				
CO_2 capture	317.45	3.47	0.61	0.02
CO_2 conversion[a]	−400.00	0.16	2.48	0.72
Displacement credits[b]	−1036.57	−4.66	−0.34	−0.22
Total	−1119.12	−1.03	2.75	0.51

[a] CO_2 conversion includes the electrolysis of water and the compression of CO_2 to 30 bar. Stoichiometric conversion processes are assumed. [b] Displacement credits are shown as negative values.

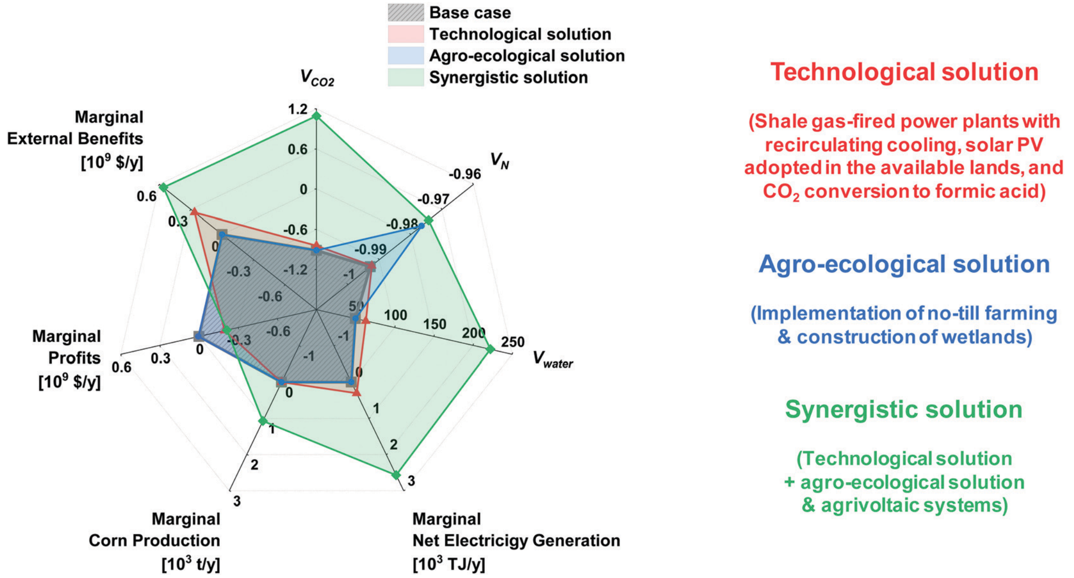


Fig. 5 Sustainability indicators for the base case, technological solution, agro-ecological solution, and synergistic solution. The available land area is utilized for employing solar PV plants in the technological solution and for constructing wetlands in the agro-ecological and synergistic solutions. The synergistic solution employs agrivoltaic systems in farmlands to generate synergy between technological and agro-ecological systems.

indicators (V_k) and an economic indicator (marginal profits). However, if the external benefits are internalized in the market, the solution can result in an increase in total profits while satisfying both human and ecosystem needs.

Depending on the regional characteristics, such as the availability of resources, climate, and market conditions, different technological alternatives may be preferred. For example, if hydraulic fracturing activities are very intense in a region, other types of fuel could be preferred to avoid or minimize the interventions from shale gas production. If a region has scarce water resources, dry cooling should be prioritized over other expensive and water-intensive technological alternatives such as CO_2 conversion. Wind power could show more benefits than solar power depending on regional climate conditions and geographic characteristics. Also, effective CO_2 conversion options and scales could vary with those regional conditions.

3.4 Techno-ecologically synergistic strategy 1: agro-ecological solution

Unlike technological alternatives whose only effect is to reduce environmental impacts or the demand for ecosystem services, agro-ecological options such as alternative farming practices and land-use change could enhance the supply of ecosystem services as well. According to the TES sustainability metrics shown in eqn (6), increasing the ecosystem service supply (S_k) helps improve the sustainability of human activities. For instance, as shown in Table 1 and Fig. S6a (ESI†), the practice of no-till farming improves the V_N indicator by reducing nutrient runoff from farming.[82] No-till farming also improves the V_{CO_2} indicator by enhancing soil carbon sequestration.[83] However, the scale of changes in these indicators is not large. In addition, marginal profits for the no-till option are slightly larger than the other tillage options despite the decreased corn productivity since it needs less labor and machinery.[84]

Also, the barren land area could potentially be reforested to provide additional forest ecosystem services, such as climate and air quality regulation. Wetlands could be constructed in the area to increase the nutrient retention service. These are ecological ways of using land to enhance the supply of ecosystem services. The V_N indicator, which most technological alternatives considered so far do not improve effectively, can be addressed by ecological land-use change. Reforestation helps to improve the V_N indicator since additional tree cover helps reduce nutrient runoff through soil infiltration.[85] However, as shown in Table 1 and Fig. S6b (ESI†), construction of additional wetlands is the most effective land-use change option to enhance the nutrient runoff indicator among any options in this study. Therefore, the V_N indicator can be improved most by employing the no-till practice and constructing wetlands on the barren lands. Detailed discussion on argo-ecological strategies, such as different tillage practices and land-use change, can be found in Section S5 (ESI†).

3.5 Techno-ecologically synergistic strategy 2: agrivoltaics

Efforts for generating more renewable energy could reduce the supply of ecosystem services. For example, filling in wetlands to install solar panels[86] could aggravate water quality and cause eutrophication by eliminating valuable ecosystem services that wetlands provide. Also, solar development in deserts has negative effects on vegetation and its ability to provide various ecosystem services.[87] TES design of renewable energy systems may address these trade-offs, and such designs are being studied for desert[10] and agricultural landscapes.[88–91] The most plausible and more sustainable solution could be the combination of solar PV and agro-ecological options by distributing the land area optimally between the alternatives. Current studies indicate that agrivoltaic systems could be attractive for synergistic generation of electricity and growth of shade-tolerant crops, such as lettuce. In the MRW, however, most of the farmlands are used for growing corn and soybeans, which are not shade-tolerant.

Several studies have examined the performance of agrivoltaic systems for shade-intolerant crops, such as grape[92] and corn.[93,94] The studies found that the effect of PV panels on crop productivity is minimal. An investigation on the performance of agrivoltaic systems on corn farming was conducted at experimental farms in Japan.[93,94] They reported that the corn yield per area was decreased by 3.6% when 0.76 m-wide PV panels were installed at the height of 2.7 m with 0.71 m intervals (high-density systems). However, when the panels were installed with 1.67 m intervals (low-density systems), the yield increased by 5.6%. The authors discussed that the increase in corn productivity could be due to the positive effects of shading caused by the panels on farm ecosystems. The shading can reduce water evaporation as well as soil erosion. Also, only a portion of sunlight is needed for the maximum rate of photosynthesis. Besides, Barron-Gafford *et al.* found that shading by the PV panels could improve the productivity of vegetation and alleviate heat stress on the panels due to latent heat fluxes between the panels and vegetation.[90] Furthermore, new technologies have been developed to reduce shading in agrivoltaic systems by employing solar tracking panels, patterned panel design, bifacial vertical panels, and semi-transparent panels.[91,93,95,96]

In this work, we consider integrated systems of solar PV panels and corn farms by employing the average of the experimental results for the low-density and high-density agrivoltaic systems.[93,94] In the MRW, if 60.9% of farmlands adopt agrivoltaic systems, they will generate the same amount of electricity from PV plants as fossil plants in the base case. Fig. 5 compares sustainability indicators between the base case, technological solution, agro-ecological solution, and synergistic solution. The technological solution refers to the solution from the CPP strategy in Section 3.3, which includes shale NGCC power plants with recirculating cooling systems, solar PV plants (with 20% module efficiency) for the available land area, and 400 000 t per year of CO_2 conversion to formic acid. The technological solution is effective for improving V_{CO_2} and V_{water} indicators, and thus, it provides large external benefits. This solution corresponds to the technology-focused solution since the available land area is allocated to the solar PV power plants. The agro-ecological solution includes the implementation of no-till practice and the construction of wetlands in the available land area. This solution shows significant improvement in the nutrient runoff indicator, V_N.

As shown in Table 1 and Fig. 5, the synergistic solution indicates an integrated solution that combines technological and agro-ecological alternatives. The available land area is utilized for wetland construction to improve the V_N indicator. Agrivoltaic systems are employed to maximize various benefits of renewable power generation (*i.e.*, smaller interventions than fossil power generation) while increasing corn productivity slightly. The improved corn yield leads to more profits, but the synergistic solution is less profitable than the base case due to expensive CO_2 conversion technologies, which enhance the V_{CO_2} indicator. As discussed in Section 3.3, however, the marginal change in total profits can be positive if the external benefits of ecosystem services are internalized in the market. Thus, the integrated solution generates synergy between technological and agro-ecological alternatives in improving multiple sustainability indicators compared to the base case. The solution can also provide greater benefits to both human and ecological systems.

4 Conclusions

Ecosystems provide various services that can be beneficial to FEW systems, industry, and society. Watershed ecosystems provide freshwater, which is one of the key resources for energy and food systems. Waste flows such as GHG emissions and nutrient releases from the FEW systems can be utilized by forest and wetland ecosystems to suppress ecological overshoot. In this sense, the FEW nexus modeling framework needs to be extended to include ecosystem and waste flows.

As opposed to the traditional FEW nexus, the TES-FEW nexus framework developed in this work can identify novel synergistic solutions that can improve food–energy–water flows while improving human well-being. This framework calculates absolute sustainability indicators to quantify the extent of ecological overshoot in the selected region. As demonstrated in this work, accounting for ecosystem services in the FEW nexus model could result in different solutions and decisions. While the traditional FEW nexus model can only identify opportunities for reducing environmental impacts, the TES-FEW nexus model can identify opportunities for improving ecosystem services as well. Moreover, the model can estimate the external benefits of ecosystem services and lead to different conclusions if the benefits are internalized in the market. Depending on the case, this may allow a 'win–win' solution for both economic and environmental indicators while meeting both human and ecosystem needs.

In this work, we focused on watershed-scale FEW systems since water is a primary element in the FEW nexus. Both the energy and food industries largely rely on the sustainable supply of water. To manage watersheds sustainably, common watershed resources such as water supply, available lands, and other ecosystem services must be distributed properly among multilateral stakeholders to enhance overall watershed functions.[18] In this context, sustainable management strategies for FEW systems should not focus on one indicator but multiple ones, including climate change, air quality, water quality, water quantity, food production, and monetary profits. We focused on CO_2, N nutrient, water quantity, corn production, and monetary indicators in this work.

As a case study, various technological and agro-ecological alternatives in the MRW were discussed using the TES-FEW nexus modeling framework. Technological alternatives were defined as the CPP strategy, which includes diverse alternatives such as NGCC power generation, water-efficient cooling technologies, renewable power generation, and CO_2 conversion technologies. Agro-ecological alternatives referred to different tillage farming practices and ecological land-use change options for the available land area. The TES-FEW nexus framework enabled us to identify the environmental effectiveness and economic feasibility of the alternatives by understanding the interactions between FEW systems and ecosystems.

Among the technological options, converting CST plants to NGCC power plants is essential for improving every sustainability indicator. Also, employing dry cooling systems is the most effective option for improving the water quantity indicator. However, dry cooling systems are costly and energy-intensive. Therefore, in regions such as the MRW, where water scarcity is not an issue, recirculating cooling makes more sense. Renewable power generation technologies such as wind turbines and solar PV panels can displace fossil fuel power plants. While installing wind turbines in the available land area results in larger monetary profits than the other power generation options, solar PV panels could be a more profitable alternative if the external benefits of mitigating impacts are internalized. In addition, CO_2 emissions can be captured and converted to formic acid. Although CO_2 conversion processes are highly energy-intensive and expensive, the internalization of external benefits could result in positive profits for a technological solution that includes employing NGCC with recirculating cooling, installing solar PV plants for the available land area, and converting CO_2 into formic acid, while effectively mitigating CO_2 emissions and water consumption.

Unlike technological alternatives, agro-ecological alternatives could enhance sustainability indicators by increasing the supply of ecosystem services. For the best nutrient indicator, the available land area should be allocated to construct wetlands, which provide the nutrient retention service. However, this ecological land-use option competes with technological land-use options, such as installing solar PV panels, which effectively improve various sustainability indicators except for the nutrient indicator. The best solution could be employing the integrated systems of technological and agro-ecological options. Therefore, in this work, we considered agrivoltaic systems for installing PV panels on corn farms while accounting for the effect of the panels on crop productivity. This solution could lead to synergy between technological and agro-ecological systems, which can improve multiple sustainability indicators. Nature-based solutions are indeed needed and should be integrated with technology-based solutions to meet multiple stakeholders' needs while respecting nature's limits.

The TES-FEW nexus takes account of FEW systems and their interactions with ecosystems. Data collection for such comprehensive analysis and design is a challenging task. In this study, we utilized various subsystem models, such as SWAT[24] and i-Tree,[25,26] and numerous data sources listed in Table S1 (ESI†). In case of lack of high-quality data and models (*e.g.*, region-specific data), low-quality data (*e.g.*, national average data) could be utilized as approximation instead, combined with uncertainty analysis. Also, stoichiometric CO_2 conversion processes were assumed since these processes are not yet commercialized. The robustness of results needs to be evaluated through sensitivity analysis of uncertain data. Moreover, other types of carbon capture technologies, such as calcium looping and piperazine-based capture, have been developed, and they perform better than the traditional MEA-based technology in terms of many characteristics.[46,97,98] Additional studies could be conducted with LCI and economic data for such technologies.

Activities in the FEW systems and ecosystems vary by season and region. For example, renewable power generation depends on season, weather, and location. Spatial and temporal analyses could be performed to gain insights into such variations in the FEW nexus. Also, the end-of-life phase of solar and wind power generation needs to be considered for a complete life cycle study.[38,39] In addition, the impacts of climate change on the nexus could be considered to ensure FEW nexus security under climate change scenarios. Moreover, a multi-spatial scale FEW nexus model could be constructed to account for different serviceshed scales of ecosystem services. Additionally, nutrient trading schemes between economic entities in the watershed could be examined to see if it can generate both economic and environmental benefits. For more robust economic analysis, market conditions (*e.g.*, investment budget and labor) and market behavior (*e.g.*, price elasticity) could be accounted for in the FEW nexus modeling work.[99] Use of sophisticated economic models such as the rectangular choice-of-technology model[100] and general equilibrium model[101–103] may be needed.

This work accounts for the function of ecosystems in addition to the traditional FEW nexus elements. The nexus approach needs to be further expanded to capture interactions between additional elements, such as those in financial, political, and social subsystems.[20,21] If such subsystems are incorporated into the nexus approach, we could better understand how each case presented in this work could be implemented and how the paradigm could shift toward a more sustainable future. We hope our work encourages such research.

Author contributions

Kyuha Lee: conceptualization, data curation, formal analysis, investigation, methodology, software, visualization, writing – original draft, review and editing. Sami Khanal: supervision, writing – review and editing. Bhavik Bakshi: conceptualization, funding acquisition, project administration, supervision, writing – review and editing.

Conflicts of interest

There are no conflicts of interest.

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