Supplementary Information 1:

Techno-Ecologically Synergistic Food-Energy-Water Systems can Meet Human and Ecosystem Needs

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S1 Data Sources

In the main paper, a case study for the TES-FEW modeling framework is conducted. Table S1 summarizes various data sources used in the case study.

Table S1: Data sources for activities, environmental interventions, and ecosystem services in the Muskingum River Watershed. If the spatial resolution of data is larger than the HUC8 scale, the data is allocated to the HUC8 scale based on the ratio of population or area.

Activities	Data Types	Data Sources	Spatial Resolution
Thermoelectric	GHG emissions	EPA eGRID[1]	Facility
	Air pollutants	EPA NEI[2]	County
	Water pollutants	EPA NPDES[3]	Facility
	Thermal water pollution	EIA-923[4]	Facility
	Water withdrawal	EIA-923[4]	Facility
	Water consumption	EIA-923[4]	Facility
	Natural gas consumption	EIA-923[4]	Facility
	Electricity consumption	EIA-923[4]	Facility
	Electricity generation	EIA-923[4]	Facility
	Cost	Multiple sources[5–7]	-
Mining	GHG emissions	GREET[8]	U.S. average
	Air pollutants	EPA NEI[2]	County
	Water pollutants	NETL[9,10]	Appalachia average
	Water withdrawal	USGS[11]	Ohio
	Water consumption	GREET[8]	U.S. average
	Natural gas consumption	EIA[12]	Ohio
	Electricity consumption	USLCI[13]	U.S. average
Agricultural & Other Activities (Residential, Commercial, Industrial, Transportation, Wastewater treatment)	GHG emissions	EPA GHGRP[1] EPA NEI[2]	Facility County
	Air pollutants	EPA NEI[2]	County
	Water pollutants	(Agricultural) SWAT[14] (Other activities) EPA[15]	HUC8 HUC4
	Water withdrawal	EnviroAtlas[16]	HUC8
	Water consumption	USGS[11]	Ohio
	Natural gas consumption	EIA[12]	Ohio
	Electricity consumption	EIA[17]	Ohio
	Food production	SWAT[14]	HUC8
	Tillage cost	Weersink et al. (1992)[18]	-
Supply of Ecosystem Services	Carbon sequestration	(Vegetation) i-Tree Landscape[19] (Soil) West and Post (2002)[20]	HUC8 -
	Air quality regulation	i-Tree Landscape[19]	HUC8
	Water quality regulation	Kadlec (2016),[21] Kadlec (2018)[22]	-
	Water provisioning	SWAT[14]	HUC8
	External benefits	EVRI[23]	-
Alternatives	Renewable power	GREET,[8] EIA[5]	-
	CO_2 conversion	Multiple sources[5,13,24–27]	-
	Land-use change	Multiple sources[28–30]	-

S2 Characteristics of Existing Activities in the MRW

S2.1 Mining of Fuel Sources

Coal was the most used fuel source for electricity generation. In the late 1980s, coal accounted for 56% of fuel sources for the U.S. energy sector.[31] However, mining and coal use result in huge environmental and health impacts. Coal was responsible for 85% of CO_2 emissions for the U.S. energy sector in the late 1980s[31] and its GHG emission intensity is more than two times larger than NG.[32] Also, air pollutants from the combustion of coal cause a lot of health problems.[33,34] Therefore, coal has been replaced in many cases by other energy sources such as NG and renewable sources. In 2018, coal accounted for only 32% of fuel sources for the U.S. energy sector.

In contrast to coal, the extraction and use of NG have continued to increase and it accounts for 29% of fuel sources for the 2018 U.S. energy sector.[31] NG accounted for only 10% in the late 1980s. The recent development of shale gas has accelerated NG exploitation. While NG is conventionally extracted by vertical and directional drilling, shale gas is extracted by horizontal drilling and hydraulic fracturing (fracking). For the past five years in the U.S., while the production of conventional NG is reduced by 41%, the production of NG from shale wells has doubled.[35] However, the hydraulic fracturing process uses a large amount of water.[36] Water resources may also be contaminated by the fracking process due to wastewater from shale wells.[37,38] This may cause harmful human and ecological health impacts. In addition, the extraction of NG will lead to volatile hydrocarbon emissions, such as fugitive methane, ground-level ozone formation, and particulate matter emissions, which may put human health at risk.[39]

Fossil fuel resources are transported from the mining sites to the power plants. Coal is transported by diesel-fueled trucks and trains, and thus, its transportation causes GHG and air pollutant emissions. On the other hand, NG is transported through pipelines at high pressure. The leakage of gas from the well site, processing, transmission, and distribution of NG results in environmental impacts.

S2.2 Thermoelectric Power Generation

Since the industrial revolution, fossil resources have been the major power sources. In 2018, thermoelectric power plants accounted for 61% of electricity in the U.S.[31] However, thermoelectric power generation is also one of the largest contributors to a variety of environmental impacts. In the U.S., thermoelectric activities accounted for 41% of water withdrawals in 2015.[40] They were also responsible for 27% of the 2017 U.S. GHG emissions,[41] 67% of the 2014 U.S. SO_2 emissions, and 12% of the 2014 U.S. NO_X emissions.[2]

Those impacts from power generation depend not only on the type of fuel but also on cooling technologies. In 2018, 34% and 59% of power plants in the U.S. were operating with once-through (OT) and recirculating (RE) cooling technologies, respectively.[4] Both technologies are wet cooling methods. The OT technology withdraws a large amount of water for cooling and discharges most of it to the watershed at a higher temperature. Thus, the OT technology causes thermal water pollution which affects water quality such as the amount of dissolved oxygen content in the water body. Due to the ecological impacts of OT technology, it has been replaced by other cooling technologies. The RE technology withdraws only a small portion of water and recirculates it. However, due to the evaporation from the cooling tower, the RE technology shows larger water consumption than the OT technology. Also, RE technology is more energy-intensive and expensive than OT technology. Loew et al. (2016) reported that the net generation efficiency is decreased by 0.3–1% and the average cost is increased by 0.12–0.27 cents/kWh if the OT technology is converted to the RE technology in the fossil power plants in Texas, U.S.[6]

Dry cooling technology does not use water since it uses air for cooling. Approximately 6% of power plants in the U.S. were operating with the dry cooling technology in 2018.[4] However, its energy generation efficiency is smaller and its cost is higher than wet cooling technologies. It was reported that the net plant efficiency is reduced by 1–4% and the average cost is increased by 0.60–0.63 cents/kWh when the RE technology in the Texas power plants is retrofitted to the dry cooling technology.[6] Also, the low energy generation efficiency results in increased emissions for generating electricity since more fuel resources need to be consumed.

S2.3 Agricultural Activities

Interventions from farming activities depend on weather conditions. If a region suffers from water shortage due to low precipitation, a large amount of water needs to be used for irrigation. Accordingly, water may need to be allocated to agricultural activities instead of other water-intensive activities such as thermoelectric activities. In such a case, technologies that do not require much water (e.g., dry cooling technology) could be preferred to minimize water consumption. If the region experiences frequent heavy rainfall, the amount of nutrient runoff from farm fields is increased.

Environmental interventions also vary with farming practices such as tillage, crop rotation, buffer strips, and cover crops. These practices affect food productivity, water nutrient emissions, soil erosion, and even ecosystem services such as carbon sequestration and soil retention. For example, tillage practices are performed to improve crop productivity. They are categorized into three practices: intensive, reduced, and conservation tillage. Intensive tillage (also called conventional tillage) has high soil mixing efficiency (uniformity) and leaves less than 15% of crop residues on the soil. Therefore, it requires large amounts of fertilizers to enhance crop yield. Accordingly, it shows an increased risk of soil erosion and eutrophication due to nutrient runoff. The reduced and conservation tillage practices have 15–30% of crop residues and more than 30% of crop residues on the soil, respectively, and thus, they show smaller soil erosion and nutrient runoff than intensive tillage. On the other hand, no-till practice shows the least risk of soil erosion and nutrient runoff, although it is likely to reduce crop yield. However, the long-term crop yield could be increased due to improved soil fertility. Also, soil carbon sequestration can be enhanced by employing no-till practice instead of tillage practices. For example, a study in Wooster, Ohio, the U.S. showed that the no-till practice can sequester 83 g $C/m^2/y$ more than conventional tillage.[20] Moreover, no-till practice is cheaper than tillage practices since it requires less labor and machinery. Weersink et al. (1992) investigated costs of no-till and various tillage practices, and estimated the average cost of no-till practice to be 7.7% cheaper than intensive tillage.[18]

S3 Muskingum River Watershed in Ohio, the United States

Figure S1 exhibits a land-use land-cover map for the Muskingum River Watershed (MRW). The map shows the watershed boundary where the 8-digits of hydrologic unit code (HUC) is 05000405. The Muskingum River in the MRW flows into the Ohio River, which flows into the Mississippi River and eventually drains into the Gulf of Mexico. Water nutrient emissions from the MRW also flow into those downstream rivers.

In 2014, the Conesville Power Plant was a coal-fired steam turbine (CST) power plant equipped with recirculating (RE) cooling systems. This coal power plant is still operating. On the other hand, the Muskingum River Power Plant which was a CST plant with once-through (OT) cooling systems was shut down in 2015 due to environmental impacts from its operation. Since the analysis in this case study is for the year 2014, we include the Muskingum River Power Plant in the analysis to maintain consistency of the data. The other three power plants in the MRW (Dresden Energy, Waterford, and Dynegy Washington) are NGCC power plants with RE cooling systems. In 2014, 48% of electricity was generated from the CST plants, and the rest 52% was from the NGCC plants.[4] For renewable energy production, the U.S. EPA's EnviroAtlas shows that solar and wind energy potentials per unit area in the MRW are 1.23 and 0.44 $MWh/m^2/y$.[16] Modern solar PV modules commercially available convert 15–20% of solar energy into electricity.[42] Common wind turbines have about 35–45% of energy conversion efficiency.[43]

In the MRW, 8.4×10^4 TJ/y of electricity is generated from five thermoelectric power plants. A CST plant with OT cooling systems (Muskingum River Power Plant) and a CST plant with RE cooling systems (Conesville Power Plant) produce 14% and 34% of electricity, respectively. The rest 52% is produced from

NGCC plants with RE cooling systems. Figure S2 exhibits the intensity of various environmental impacts for three types of power plants in the MRW. All values are normalized by total electricity generated in the MRW (TJ_{elec}). Compared to the CST plants, NGCC plants show smaller intensities for every impact category. In comparison between OT and RE cooling technologies, CST with RE shows higher CO_2 and NO_X emissions than CST with OT (Fig. S2 (a) and (b)). This is because the RE systems have lower power generation efficiency than the OT systems. With respect to SO_2 emissions, however, CST with RE shows much lower emissions than CST with OT because of the flue gas desulfurization (FGD) systems in the CST plant with RE (Conesville Power Plant) (Fig. S2 (b)). The CST plant with OT (Muskingum River Power Plant) was not equipped with FGD systems in 2014 and was one of the largest SO_2 emitters in the nation.[4] Also, CST with OT withdraws more water than CST with RE, while the amount of water consumption is higher for the RE systems than the OT systems due to evaporative losses from the cooling tower (Fig. S2 (c)). However, OT systems result in huge thermal water pollution due to the cooling water discharge to the watershed, which leads to damages to the watershed ecosystems.

As shown in Fig. S1, the MRW had 3.76×10^8 m^2 of farmland (9.24% of land-use in the MRW). Production of corn and soybean was 2.2×10^5 t/y and 7.2×10^4 t/y, respectively. 57.0% of tillage practices in the MRW were no-till practice, while 22.29%, 20.0%, and 0.11% of the practices were conservation, reduced, and intensive tillage practices, respectively. Wetlands and forests accounted for 0.14% and 57.45% of land-use, respectively. The MRW also had 1.30×10^7 m^2 of barren land (0.32% of land-use). In this work, the status of FEW systems in the MRW for the year 2014 is defined as the base case.

S4 Additional Discussion about Technological Strategies

S4.1 Replacement of Coal by NG for Power Generation

In this work for the MRW, coal is a dirty fuel in every way, as shown in Fig. S2. Therefore, NG could be employed for a fossil power source instead of coal to improve the sustainability of power generation. Figure S3a compares various sustainability indicators among coal, conventional NG, and shale NG as fossil power sources.

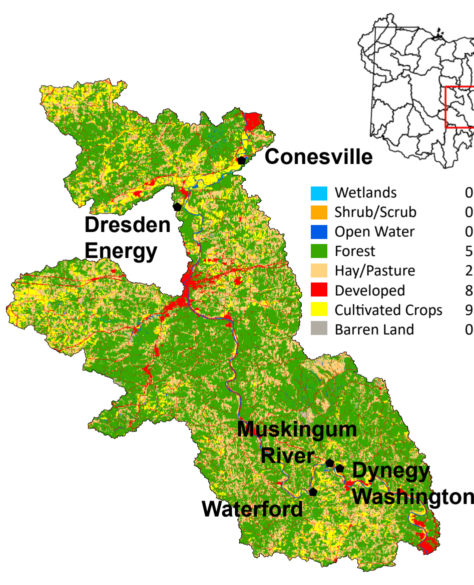


Figure S1: Land-use land-cover map for the Muskingum River Watershed (MRW). The MRW is located in the southern east of Ohio, the United States (⬟: location of thermoelectric power plants.)

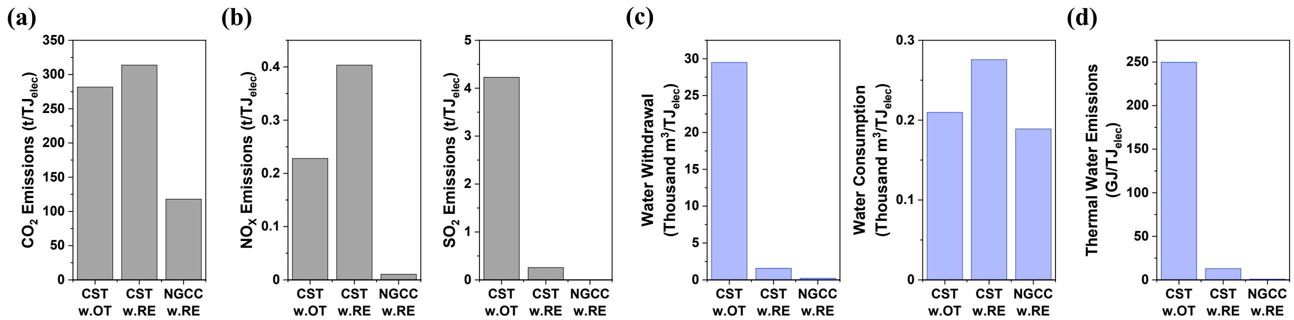
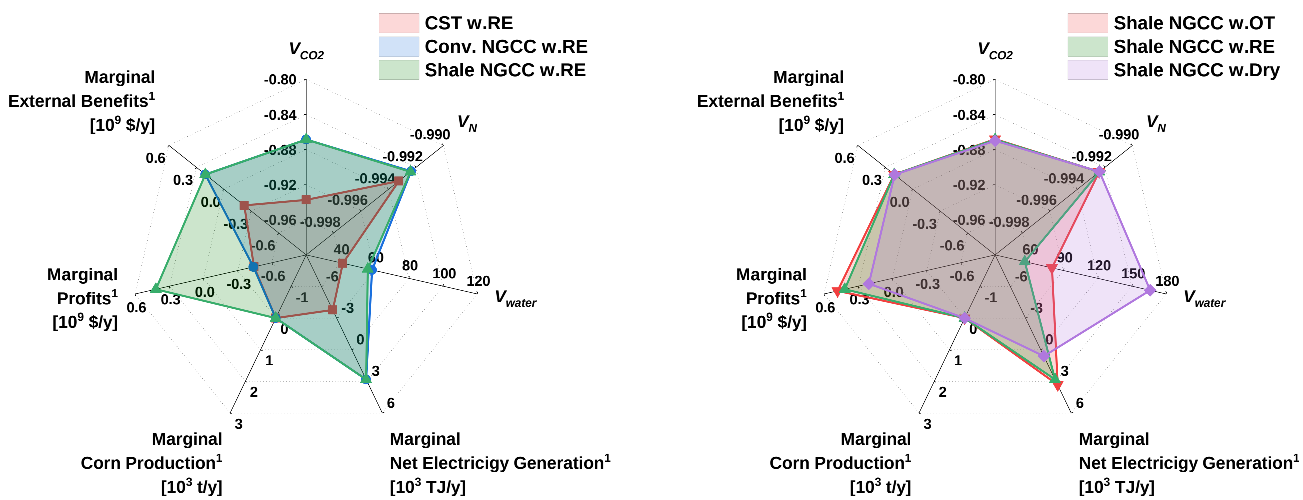


Figure S2: Intensity of environmental impacts for a CST plant with OT (Muskingum River Power Plant), a CST plant with RE (Conesville Power Plant), and NGCC plants with RE cooling systems (Dresden Energy, Waterford, and Dynegy Washington Power Plants) in the MRW. **(a)** GHG emissions, **(b)** air pollutant emissions, **(c)** water use, and **(d)** thermal water emissions.



(a)

(b)

Figure S3: Sustainability indicators for **(a)** different fuel options for generating electricity and **(b)** different cooling technology options for generating electricity. These indicators are defined such that larger values indicate greater sustainability. Note that the scale of V_{water} axis is different in each plot. Shale NGCC with RE and shale NGCC with dry cooling are desirable for water-affluent and water-scarce regions, respectively. [1]Marginal values are based on comparison with the base case.

S4.2 Water-efficient Cooling

Figure S2 exhibits that once-through (OT) cooling systems have massive thermal water emissions due to the huge amount of water discharged to the watershed at a warmer temperature, although they are energy efficient and economically cheaper than other cooling technologies. We compare three cooling systems (OT, RE, and dry cooling) by assuming that all five fossil power plants in the MRW adopt the same type of cooling systems. As shown in Fig. S3b, dry cooling systems can be very effective for improving the TES water sustainability indicator (V_{water}) since they do not require the use of water for cooling. However, dry cooling is more energy-intensive and more economically expensive than wet cooling options. For water-scarce regions that have a negative V_{water} value, the dry cooling technology could be a good alternative to improve water sustainability.

S4.3 Renewable Power Generation

The previous results in Fig. S3 show that the shale NGCC plants with recirculating (RE) systems are preferred for the MRW in both environmental and economic aspects. Solar PV (with 15–20% module efficiency) and wind power (with 35–45% energy conversion efficiency) plants could be adopted to the available barren lands to replace 7.2–9.6% and 0.3–0.4% of electricity produced from the shale NGCC plants with RE systems, respectively. Table S2 exhibits sensitivity analysis results with respect to the range of energy conversion efficiency of renewable power generation technologies. The results are robust regardless of the conversion efficiency.

Figure S4a exhibits sustainability indicators for adopting solar PV (with 20% module efficiency) and wind power (with 45% energy conversion efficiency) plants to the available barren lands. Renewable power plants do not require an electricity input in generating electricity, while fossil power plants have some parasitic energy losses (e.g., NGCC plants with RE systems in the MRW require 0.02 J of electricity to generate 1 J of electricity[4]). Thus, renewable options show higher marginal net electricity generation values than fossil options.

With respect to monetary aspects, if we only consider profits for the private sector, employing the wind power option makes sense due to its lower levelized costs of electricity (LCOE). On the other hand, if the external benefits are internalized, the solar power option should be favored to maximize total profits (i.e., the sum of marginal profits made by companies and marginal external benefits to society). In this case, sticking to using shale NGCC plants is the most expensive option because of its lower external benefits than the renewable options. The U.S. EIA report also estimates that the LCOE for solar PV and wind power technologies can be cheaper than the NGCC technology if federal tax credits to promote the use of renewable technologies are included.[5]

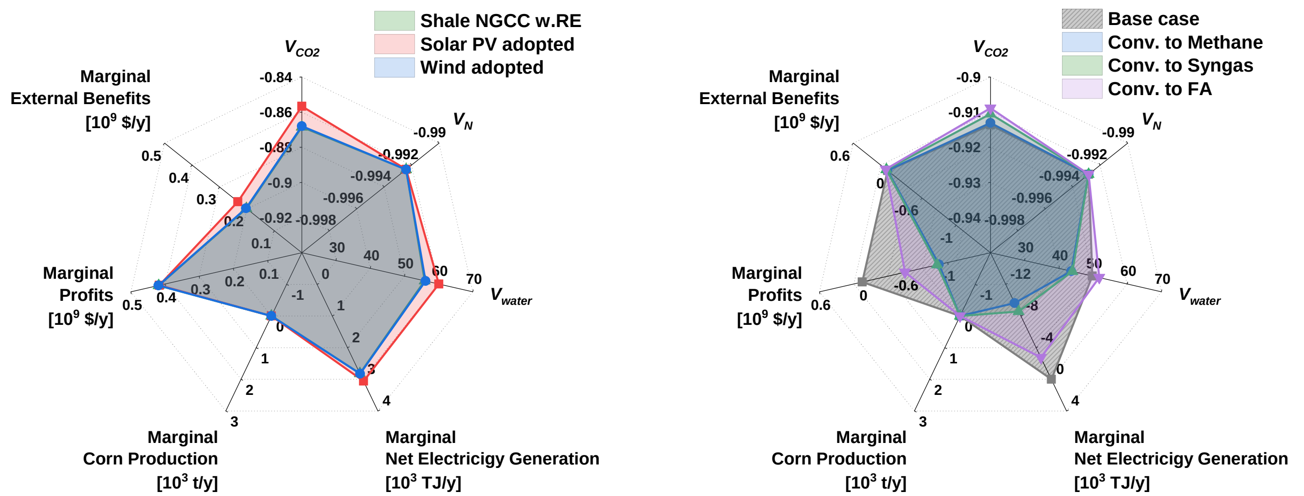
S4.4 CO_2 Conversion

Sustainability indicators for three conversion options are shown in Fig. S4b. The formic acid option is more lucrative than the other conversion options. This is not only because the formic acid conversion option is less energy-intensive, but also because the monetary displacement credits from the conventional formic acid process are large. In other words, Prod_{elec} in Eq. 9 for the formic acid option is larger than the other options. Also, $\text{Cost}_{formic\ acid}$ in Eq. 9 for the formic acid option is smaller than the other options because of the higher displacement credits, as shown in Table 2.

Due to the limited demand for CO_2 converted products, the production scale of CO_2 conversion is limited. For example, 400,000 t/y of CO_2 conversion to formic acid corresponds to 57% of the global production capacity for formic acid in 2013 (697 thousand t).[27] It is less likely to be able to utilize CO_2 to produce formic acid in the MRW. However, market conditions have been changing over the years.

Table S2: Sensitivity analysis results for adopting renewable power plants (solar PV or wind power) to 1.30×10^7 m^2 of barren lands to replace shale NGCC power plants with RE systems. The range of energy conversion efficiency (15–20% of PV module efficiency and 35–45% of wind turbine efficiency) is considered. [1]V_k metrics represent absolute sustainability with respect to k-th flow. [2]Marginal values are based on comparison with the base case. [3]External benefits correspond to the monetized benefits of ecosystem services to society.

Alternatives	V_k metrics[1]			Marginal values[2]		
	CO_2	N	Water	Net E. Gene. (10^3 TJ/y)	Profits (Million $/y)	Ext. Benefits[3] (Million $/y)
Shale NGCC w.RE	-0.8684	-0.9924	55.95	2.814	418.4	201.7
Solar PV adopted (15% module efficiency)	-0.8598	-0.9924	61.99	2.994	417.2	225.3
Wind adopted (35% turbine efficiency)	-0.8680	-0.9924	56.10	2.822	418.8	202.8
Solar PV adopted (20% module efficiency)	-0.8567	-0.9924	60.05	3.054	416.8	233.2
Wind adopted (45% turbine efficiency)	-0.8679	-0.9924	56.14	2.825	418.9	203.1



(a) (b)

Figure S4: Sustainability indicators for **(a)** adopting renewable power plants (solar PV or wind power) to 1.30×10^7 m^2 of barren lands to replace shale NGCC power plants with RE systems and **(b)** employing CO_2 conversion technologies. Note that the scale of many axes is different in each plot. Environmental indicators can be improved by employing solar PV plants and converting CO_2 into formic acid, although CO_2 conversion is costly.

According to the more recent market report,[44] the global production in 2016 was 1,015 thousand t and was expected to increase to 1,217 thousand t by 2022. In case of the methane and syngas options, they are rarely constrained given the extensive uses of NG and syngas in the market. However, their CO_2-converted products are less profitable than CO_2-converted formic acid.

The expensive production cost for CO_2 conversion processes is another constraint to employ the conversion technologies. For instance, Agarwal et al. (2011) discussed that negative net present value for the CO_2-converted formic acid is estimated over 10 years due to the high capital equipment investment cost.[45] They claimed that the profitability for the CO_2 conversion processes can be improved by technological development. In this work, we compare marginal profits and marginal external benefits among three conversion options with the varied CO_2 conversion scale when the conversion options are employed with other technological alternatives, which include shale NGCC plants with RE cooling and solar PV plants (with 20% module efficiency) in the available lands (Fig. S5). Marginal Profits represent the change in profits made by corporations by employing alternative options, while marginal external benefits correspond to the change in environmental external benefits to society. Due to the expensive cost and high energy requirement for CO_2 conversion processes, all the options become less profitable as more CO_2 is converted. When there is no CO_2 conversion, the marginal profits are positive because the solar PV power plants adopted with shale NGCC power plants with RE systems are economically beneficial than the base case, which has two coal power plants without any renewable power plant.

The marginal profits become negative when 200, 200, and 300 thousand t/y of CO_2 are converted to methane, syngas, and formic acid, respectively. That is, plant operators will have monetary losses compared to the base case profits when the above amounts 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 (marginal profits + marginal external benefits) can be positive for 200, 200, and 400 thousand t/y of CO_2 conversion to methane, syngas, and formic acid, respectively.

Most CO_2 conversion technologies are still in the research and development stage. Therefore, it is difficult and challenging to compare different CO_2 conversion options whose processes have not been optimized yet. Due to this reason, stoichiometric conversion reactions are assumed in this study. The

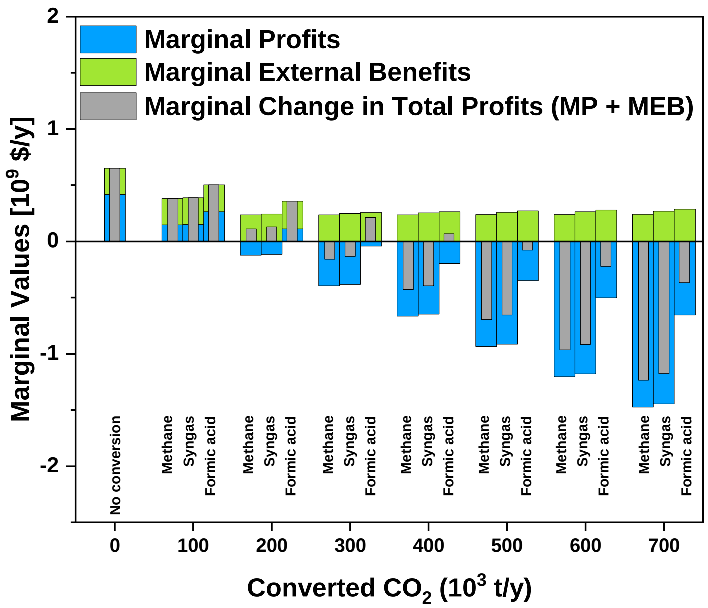


Figure S5: Marginal profits and marginal external benefits for CO_2 conversion options along with the different scale of CO_2 conversion. Due to the expensive cost of conversion technologies, profits are decreased substantially, and external benefits are increased slightly as the scale of conversion becomes larger. Marginal change in total profits can be positive when 400 thousand tCO_2 is converted to formic acid.

commercialized conversion processes are likely to have more emissions and resource use. Accordingly, their sustainability indicators will drop to some extent. Nonetheless, we could obtain some important insights into how much the conversion technologies would be effective and which options would make more sense to employ than others.

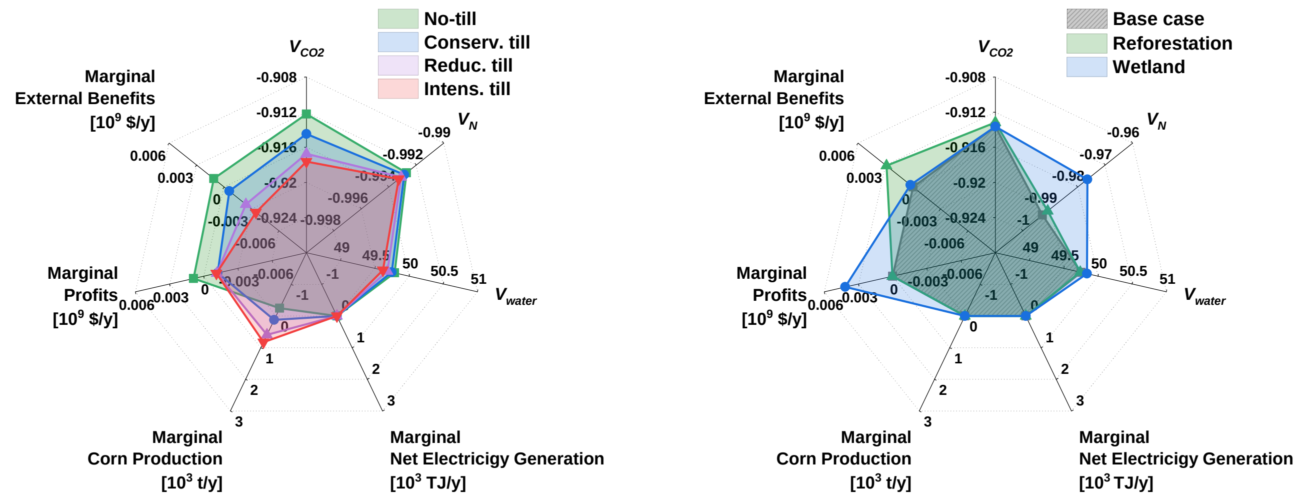
S5 Additional Discussion about Agro-ecological Strategies

S5.1 Tillage Practices

Figure S6a shows sustainability indicators for adopting four different tillage practices: no-till, conservation tillage, reduced tillage, and intensive tillage. Overall, the indicators do not vary drastically with tillage options. The no-till practice reduces corn production by 0.5% compared to intensive tillage practice. However, since the no-till practice is cheaper than the tillage practices,[18] its marginal profits are slightly larger than the other tillage options despite the decreased productivity. In addition, nutrient trading schemes could be examined to obtain a 'win-win' solution.[46] According to the scheme, other economic entities whose emissions are more expensive to abate than farming could pay farmers for credits to implement agricultural practices that result in lower food production but fewer nutrient emissions. This could yield stronger economic and environmental benefits.

S5.2 Land-use Change

The barren land area could potentially be used for various useful ways. Figure S6b exhibits ecological land-use change options for 1.30×10^7 m^2 of the barren land area in the MRW. Ecological options provide additional ecosystem services such as carbon sequestration service from the reforestation option and freshwater provisioning/nutrient retention services from the wetland option. The reforestation and wetland options improve V_{CO_2} and V_{water} indicators to a small extent, although these options are not as



(a)

(b)

Figure S6: Sustainability indicators for **(a)** employing different tillage practices and **(b)** adopting different land-use change options. Note that the scale of V_N axis is different in each plot. V_N indicator can be improved by implementing no-till practice and constructing wetlands.

effective as technological options. As depicted in the previous section, technological alternatives, such as installing solar PV plants, are much more effective to improve V_{CO_2} and V_{water} indicators.

Although the V_N index of the wetland option is still very negative, the index is increased to -0.976 from -0.993 of the base case. The negative index means the nutrient emissions in the MRW exceed the supply of nutrient retention services from the wetlands in the MRW. The excess nutrient emissions will flow into the the Muskingum River and contribute to eutrophication.

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