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Jin, E., Jabarivelisdeh, B., Meng, F. et al. (2026) Exploring pathways to achieve net-zero emissions in high-value chemical production: balancing energy, emissions, and economic considerations. ACS Sustainable Chemistry & Engineering, 14 (30). pp. 13517-13532. ISSN: 2168-0485

https://doi.org/10.1021/acssuschemeng.6c03082

ACS Sustainable Chemistry & Engineering

pubs.acs.org/journal/ascecg

Research Article

Exploring Pathways to Achieve Net-Zero Emissions in High-Value Chemical Production: Balancing Energy, Emissions, and Economic Considerations

Enze Jin, Banafsheh Jabarivelisdeh, Fanran Meng,* Phillip Christopher, and Eric Masanet

Cite This: *ACS Sustain. Chem. Eng.* 2026, 14, 13517−13532

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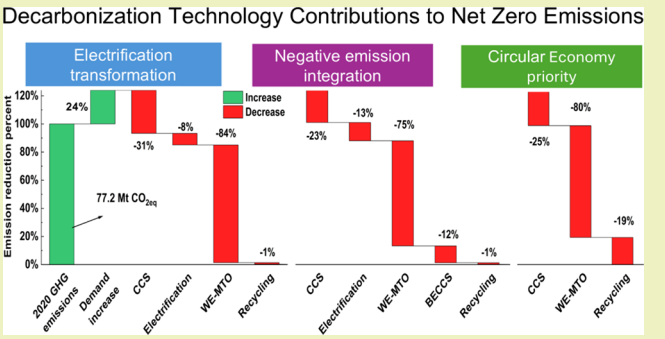
ABSTRACT: High-value chemicals (HVCs) are the main intermediate chemical building blocks for producing goods such as plastics, tires, and other products, contributing 18% of U.S. chemical industry emissions in 2020. However, there is limited robust guidance on decarbonizing this sector. This study explores cost-effective pathways for achieving a net-zero U.S. HVC industry by 2050, and key strategies include ethane cracking electrification with renewable energy, mechanical recycling, bioethanol dehydration, and carbon capture. We demonstrate that while current IRA policies are insufficient alone, a high circular economy pathway, reaching 50% recycling by 2030, offers the least system costs, mitigating 1.48 Gt CO_{2eq} and reducing energy demand by 0.11 EJ relative to no-mitigation baselines. Furthermore, we conclude that integrated system optimization is more cost-effective than product-specific decarbonization, provided that residual upstream emissions are addressed via sector-integrated negative-emission technologies. This analysis also indicates that reducing emissions from upstream petrochemical feedstock is essential for easing the decarbonization burden on the HVC industry.



KEYWORDS: *high-value chemicals, ethylene, climate change, energy systems modeling, plastics, carbon tax credit, Inflation Reduction Act*

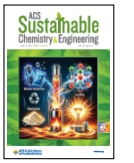
INTRODUCTION

The global net-zero emission goal by 2050 has been set by energy and climate policies to limit the global mean temperature increase to 2 °C or even 1.5 °C relative to the pre-industrial era. A recent study from the Indicators of Global Climate Change (IGCC)[1] pointed out that the remaining 1.5°C carbon budget of 130 Gt CO_{2eq} at the beginning of 2025 would be exhausted in over three years based on the current global emissions rate of 40 Gt CO_{2eq} estimated by the Intergovernmental Panel on Climate Change (IPCC) Sixth Assessment Report.[2] Therefore, it is extremely urgent to decarbonize future emissions caused by human activities.

U.S. chemicals production and oil refining contribute ∼8% to gross domestic product (GDP) and are critical for U.S. energy security.[3] The chemicals and petrochemicals industry is one of the most energy-intensive industries and is the major contributor to the total emissions of the industrial sector, which emitted 233 million metric tons of CO_{2eq} in 2021, accounting for ∼4% of total CO_2 emissions and 17% of total industrial emissions.[3]

Today, the U.S. chemical sector produces around 40% of global ethane-based petrochemicals by mass.[4] High-value chemicals (HVC), including ethylene, propylene, benzene, toluene, and xylene (BTX), are the main intermediate chemical building blocks for plastics, tires, and other chemical products, accounting for US$153 billion U.S. market value.[3] The total production amount of HVC is 41.4 million metric tons in 2020, accounting for 18% (41 million metric tons) of the total emissions of the U.S. chemical industry. Certain ethylene production routes produce propylene as a byproduct with a 2–17%[5] output share depending on feedstocks and operations; thus, considering interconnections in designing decarbonized manufacturing scenarios is important. The major technology routes for producing HVCs in the U.S. are stream cracking using ethane or naphtha as feedstocks. In contrast to methanol and ammonia production, the emissions of HVC manufacturing processes are mainly generated from fuel combustion. Therefore, one of the promising levers to decarbonize HVC production is switching from fossil fuels to clean fuels or to electrification with renewable

Received: March 15, 2026
Revised: June 9, 2026
Accepted: June 9, 2026
Published: July 20, 2026



https://doi.org/10.1021/acssuschemeng.6c03082
ACS Sustain. Chem. Eng. 2026, 14, 13517−13532

electricity. Other levers, such as carbon capture and storage (CCS), negative emission technologies, and recycling technologies for waste plastics, can potentially play important roles in the deep decarbonization pathway for the HVC industry. Moreover, given varying interconnectedness depending on production technologies, integrated HVC systems must be considered in optimal paths to decarbonization.

Previous studies[6−13] have investigated net-zero emission pathways for global and regional chemical sectors, including ammonia, methanol, HVCs and other petrochemicals. However, a specific evaluation of the technology shifts necessary to achieve a net-zero HVC sector in the U.S. has yet to be conducted, particularly accounting for the complex technical characteristics of HVC production technologies. Furthermore, previous studies have lacked in-depth explorations for potential net-zero emission pathways under various scenarios with different plausible assumptions regarding technology innovation, cost-effectiveness, and policy levers. In addition, previous studies did not investigate potential pathways under different modeling options in terms of carbon mitigation targets and decarbonization strategies, which could significantly influence the trajectory of technology transitions.

This study aims to identify the potential technology transition pathways for achieving a net-zero HVC sector in the U.S. and to evaluate the resilience of these pathways against various technical, economic, and political variations. The study extends the existing literature in several ways. First, this study employs a detailed energy systems model incorporating rich technology resolution to identify the potential cost-effective technology transitions for achieving a net-zero HVC sector in the U.S., especially considering upstream emissions from oil and gas refineries in the carbon system boundary. Second, the model examines potential net-zero pathways associated with energy, climate change, and cost trade-offs under different plausible assumptions for future technology development, economic conditions, and policy interventions. Finally, this study includes a variety of possible decarbonization strategies from different system perspectives, including assessing the impacts of various carbon mitigation goals and delayed zero-emission technology transition situations.

In this study, net-zero pathway scenarios were generated in the TIMES (The Integrated MARKAL-EFOM System) model,[14] which aimed to understand variations in possible net-zero pathways arising from plausible changes in technical performance, economic costs, and policy interventions. Details of the approach used in the TIMES model are described in the Model overview section, with detailed scenario descriptions available in the Results section. This study makes three primary contributions: (1) it provide a robust high-resolution technology assessment of the U.S. HVC sector that integrates upstream refinery emissions into a net-zero framework; (2) it quantifies the economic and energetic trade-offs across ten distinct technical and political scenarios, identifying the indispensable role of negative-emission pathways; and (3) it evaluates the efficacy of current U.S. policy (IRA), offering actionable insights for stakeholders on the policy extensions required to incentivize a cost-effective industrial transition.

MATERIALS AND METHODS

Model Overview

This study employed the TIMES (The Integrated MARKAL-EFOM System)[14] model to simulate the net-zero emission scenario pathways for U.S. HVC production. Figure 1 depicts the adjusted TIMES model framework for the U.S. HVC system. The TIMES model has also been widely used for energy and environmental policy assessments, including for the United Nations Sustainable Development Goals and Europe Emissions Trading System (EU-ETS). This study compiled a comprehensive technology database for HVC production with detailed techno-economic parameters in the US. The database is then incorporated into the TIMES model of the net-zero emission pathways under various scenarios with plausible technical, economic, and political assumptions.

Optimization in TIMES

TIMES is a technology-rich, bottom-up model using linear programming to minimize the system costs for the energy system under user constraints on energy demand, carbon emissions, etc. over a certain time horizon. TIMES model can integrate all the processes for primary resource generation, energy commodity transformation, distribution, and conversion into the supply of HVCs to fulfil the demand by other sectors.[14] The key inputs of the HVC TIMES model include a technology dataset with technical and economic data, energy price cost data, demand projection, and other generic system data (e.g., discount rate, time periods).

The governing equations for optimizing the system costs in TIMES model are listed as below:[14]

$$NPV = \sum_{r=1}^{R} \sum_{y \in YEARS} \left(1 + d_{r,y}\right)^{REFYR-y} \times ANNCOST_{(r,y)} \quad (1)$$

where NPV is the net present value of the total cost for all regions; $ANNCOST_{(r,y)}$ is the total annual cost in region r and year y; $d_{r,y}$ is the general discount rate; $REFYR$ is the reference year for discounting; $YEARS$ is the set of years for which there are costs (in the horizon, plus past years before the beginning of the horizon); R is the set of regions in the area of study.

The objective function of TIMES model is to minimize the regional system NPV. The $ANNCOST$ of the objective function is calculated by total annual costs minus revenues (see eq 2).[15]

$$\begin{aligned} \text{Min } REG_{OBJ(y_0,r)} = \sum_{y \in YEARS} DISC_{(y,y_0)} \times \{ & INVCOST(y) + \\ & INVTAXSUB(y) + INVDECOM(y) + FIXCOST(y) + \\ & FIXTAXSUB(y) + SURVCOST(y) + VARCOST(y) + \\ & VARTAXSUB(y) + ELASTCOST(y) - \\ & LATEREVENUES(y)\} SALVAGE(y_0) \end{aligned} \quad (2)$$

where $CAPEX$ is the investment costs for installing new processes (e.g., US$/t-HVC); $INVTAXSUB$ is the taxes or subsidies on investments; $INVDECOM$ is the capital costs linked to decommissioning of a process; $FIXEDOPEX$ and $VAROPEX$ are fixed and variable operating and maintenance costs (e.g., US$/t-HVC) for processes, respectively; $FIXTAXSUB$ and $VARTAXSUB$ are the fixed and variable annual taxes and subsidies, respectively; $SURVCOST$ is the surveillance cost of the facility during the lag time before its demolition; $ELASTCOST$ is the cost incurred when demands are reduced due to price elasticity (this parameter has no impact in our model due to an increasing demand projection); $LATEREVENUES$ is the late revenues from the recycling of materials from dismantled processes that occur after the end-of-horizon; $SALVAGE$ is the salvage value of investments and other one-time costs and it is discounted to the base year y_0. In this study, there is no $ELASTCOST$ and $LATEREVENUES$ incurred.

Meanwhile, the regional HVC products produced from all production technologies have to meet the regional HVC demand as the constraint shown in eq 3.[15] In the core NZE and NZE variant scenarios,

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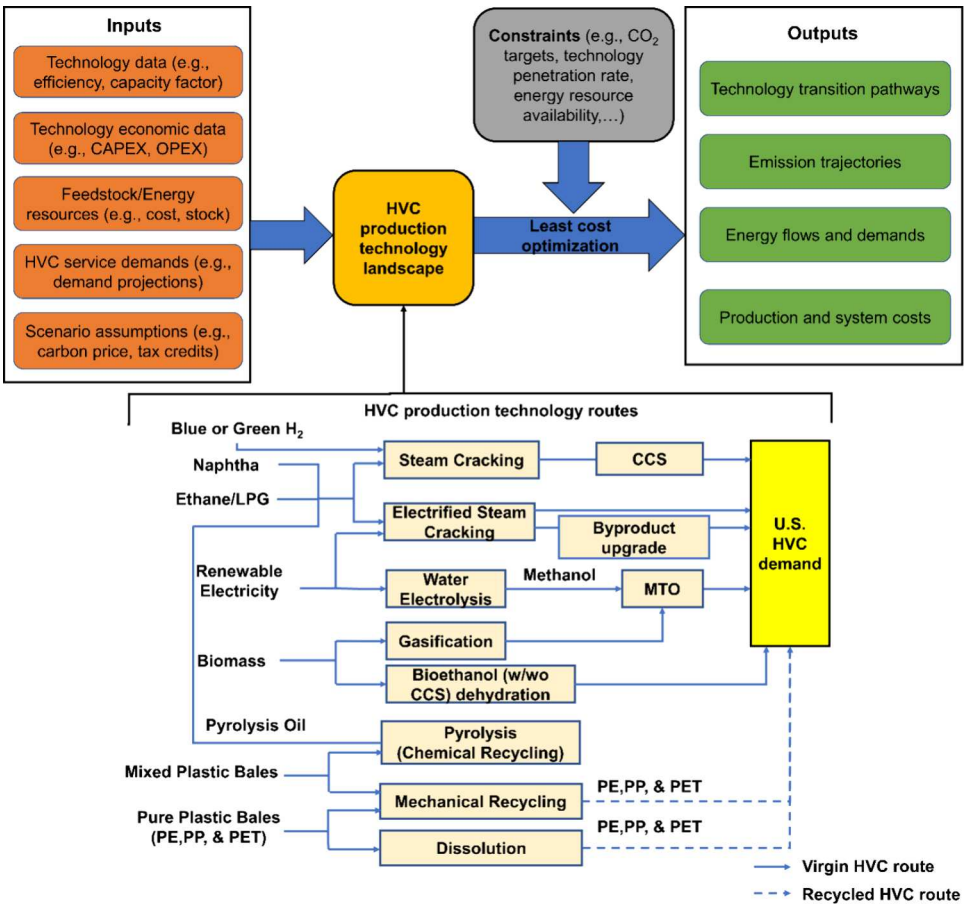

Figure 1. TIMES model framework for the U.S. HVC production.

the objective function should also be constrained by the carbon emission upper bound for each time period.

$$\Sigma VAR\_COMNET_{(r,t,c,s)} = DEMAND \quad (3)$$

where *VAR_COMNET* is the net amount for commodity *c* produced by all technologies in region *r* in each period *t* and time slice *s*. It is equal to the total import plus production and minus export; *DEMAND* is the total demand of commodity *c* in each time period *t*.

Other key equations and details are included in the Supporting Information.

HVC Production Technology Routes

The following HVC production pathways were considered in this analysis.

Conventional Pathways. Steam cracking: Steam cracking using ethane and naphtha as feedstock is the major technology for producing HVCs in the U.S. In the ethane steam cracking process, the yield of HVCs is 50% more than a naphtha-based one and the mix of HVCs produced is predominantly composed of ethylene.[4] In the naphtha steam cracking process, the yield of HVCs is more balanced with ethylene, propylene and BTX aromatics. Around 80% of HVCs are produced through ethane steam cracking in the chemical sector.

Propane dehydrogenation: Propane dehydrogenation can produce propylene as a single product. This technology has gained attention in the U.S. in recent years. Currently, the production capacity of propane dehydrogenation plants is around 2.4 million metric tons per year.

Alternative Low-Emission Pathways. Electrified steam cracking: Electrification of steam crackers with clean power can reduce significant amounts of emissions in the process. This technology has been validated, but it will take a few years to be commercialized on a large scale.[16] E-crackers powered by renewable electricity from wind and solar energy are assumed to emit zero CO_2 in this study. In the conventional steam cracker, the fuel gas of the process can be reused as fuel in the furnace.[17] In the e-cracker, fuel gas can be synthesized into methanol first and further converted into HVCs through methanol-to-olefin technology.[18]

Hydrogen-fueled steam cracking: Using hydrogen to fuel the steam cracker is another alternative way to reduce CO_2 emissions from combustion.[19,20] This study only considers blue hydrogen from steam methane reforming with CCS and green hydrogen from water electrolysis powered by renewable electricity that can be used to fuel the steam cracking process. In this study, we assume a carbon capture rate of 90% for blue hydrogen production processes. Critically, our system boundary includes upstream fugitive methane emissions associated with natural gas extraction and transport, which are integrated into the total life-cycle emission factors for blue hydrogen. It should be noted that uncertainties regarding achievable real-world carbon capture rates and the intensity of diffuse methane emissions can significantly alter the perceived decarbonization potential of blue hydrogen.

Methanol to olefins (MTO): Methanol to olefin technologies have been commercialized in China to produce ethylene and propylene using methanol as feedstock.[21] Methanol production can be decarbonized by water electrolysis powered by renewable electricity and biomass gasification. The source of carbon for the water electrolysis-based methanol is from captured CO_2 from industrial point sources (e.g., exhaust stacks of cement, steel, and ammonia manufacturing or

https://doi.org/10.1021/acssuschemeng.6c03082
ACS Sustain. Chem. Eng. 2026, 14, 13517−13532

power plants). This study only considers water electrolysis-based MTO and biomass-based MTO for ethylene and propylene. The yield ratio of ethylene to propylene in the MTO process ranges from 0.6 to 1.3.[22]

Bioethanol dehydration: Ethylene can be produced via the bioethanol dehydration process over an alumina catalyst in a fluidized bed reactor.[21] Bioethanol dehydration can be seen as a negative emission technology for ethylene when bioethanol production is decarbonized by CCS technologies. This study uses corn ethanol as a feedstock for this biobased technology. It should be noted that biobased technologies could have positive emissions depending on the crop species, harvest methods, soil carbon effects, necessary fertilization, and growth back time.

Mechanical recycling: Mechanical recycling mainly involves processes of sorting, shredding, washing, and extrusion of post-consumer plastic.[23] Mechanical recycling is applied for both mixed and pure sorted plastics. Mixed or pure sorted plastics reprocessed by mechanical recycling can be used directly without significant changes to their chemical composition in plastic manufacturing plants.[24]

Dissolution: Dissolution is a physical process in which a polymer is dissolved in a solvent and precipitated and purified by the addition of an antisolvent.[23] Similar to mechanical recycling, the dissolution process can recycle sorted plastics without changing their chemical composition, but it is only applicable to pure sorted plastics, such as HDPE, LDPE, and PET. Mechanical recycling and dissolution processes do not produce HVC monomers; instead, they provide secondary polymers that substitute for virgin materials. In this study, we quantify the impact of these technologies by estimating the savings of virgin ethylene, propylene, and BTX that would otherwise be required for polymer production.

Chemical recycling (Pyrolysis): Chemical recycling processes post-consumer plastics to intermediate chemicals by changing their chemical structure. Pyrolysis is one of the most promising recycling technologies with high feedstock flexibility and tolerance of contamination.[25] Pyrolysis can thermochemically decompose pretreated plastic waste to monomers or other chemicals that can be used as secondary feedstock in plastic or other chemical production.[24,25] This study only considers pyrolysis as a chemical recycling technology and gasification or partial solvolytic recycling due to their low technology readiness levels.[24]

Assuming a total asset lifetime of 35 years, the average remaining lifespan of existing U.S. steam cracking and propane dehydrogenation facilities is 20 years, and they will start retiring gradually after 2035. Two other classes of low-carbon technology were screened and excluded from this study. Tables S1 and S2 summarize the datasets (costs, energy and emissions intensities, etc.) used in the TIMES model for each considered technology pathway. Current technology readiness levels (TRLs) are mapped to the assumed years when the technology is available for deployment in the TIMES model.

Scenario Descriptions and Assumptions

To identify the feasible decarbonization technology transitions for a net-zero U.S. HVC sector, it is important to accurately characterize the technical and economic performance of conventional and advanced low-emitting technologies. The decarbonization technology levers of HVC production can be categorized into fuel switching (e.g., clean hydrogen-fueled ethane cracking), feedstock substitution (e.g., methanol to olefins (MTO) and mechanical recycling of sorted plastics), carbon capture and storage (CCS), and negative emission technologies (e.g., water electrolysis-based MTO). They were chosen based on existing or likely commercial availability for meaningful deployment by 2050. Detailed technical and economic parameters of technologies considered in the model are provided in Tables S1 and S2 in Supporting Information. Based on the technology dataset used in this

Table 1. Summary of Modeling Scenarios

scenario (Abbr.)	description
basic cases	
no carbon constraint (NCC)	no emission reduction constraint is implemented within the model. The role of carbon mitigation policies is overlooked.
net-zero emissions (NZE)	carbon emissions reduction target will be net-zero (100% reduction compared to the 2020 level) by 2050, inclusive of upstream fugitive GHG emissions from oil and gas refineries.
NZE variants	
NZE with enhancing BECCS utilization (NZE-BECCS)	decarbonizing bioethanol production by implementing CCS technologies (reduced by 23.8 kg CO_{2eq}/GJ).[31] The cost of bioethanol production with CCS will increase by US$1.88/GJ.[32]
NZE with enhancing green hydrogen utilization as a fuel source for cracking processes (NZE-GreenH_2)	green hydrogen will be produced at a large scale by water electrolysis powered by renewable electricity and the cost of green hydrogen will be US$1/kg by achieving the clean hydrogen goal in the U.S. under financial supports.
NZE with enhancing recycling technologies under a high circular economy circumstance of waste plastics (NZE-HighCE)	a 50% recycling rate of waste plastics will be achieved by 2030 to comply with the national goal, which will determine the maximum availability of sorted and mixed plastics for reprocessing.
NCC variants	
NCC with carbon pricing (NCC-CP)	carbon prices (US$50–500/t CO_{2eq}) are implemented to reduce the cost competitiveness of emission-intensive fossil fuel-based technology routes.
NCC with current and extended IRA Section 45Q tax credits (NCC-45Q or 45Q extension)	Section 45Q tax credits of US$85/t-$CO_{2eq}$ by 2033[33] or extended to 2050 for carbon capture and storage are implemented to promote deployment of CCUS technologies.
NCC with current and extended IRA Section 45V tax credits (NCC-45V or 45V extension)	Section 45V tax credits up to US$3/kg H_2 by 2033[34] or extended to 2050 for clean H_2 production are implemented to promote deployment of water electrolysis-based MTO technology for HVCs.
system variations	
net-zero emissions excluding upstream fugitive emissions (NZE-EUE)	only direct (combustion and process) and indirect (electricity generation-related) emissions are considered for the net zero emission target, while upstream fugitive emissions from fuel and feedstock acquisition are excluded.
net-zero emissions for each HVC product separately (NZE-Separate)	deeply decarbonize HVC production separately instead of as an integrated system.
various carbon constraints (VCC)	carbon emissions reduction target will be varied from 30 to 100% by 2050.
net-zero emissions with delayed transition starting years (NZE-PTSY)	deeply decarbonize the HVC sector with delayed transition starting years of 2025, 2030, and 2035 assuming the system faces a delayed advanced technology maturity situation.

https://doi.org/10.1021/acssuschemeng.6c03082
ACS Sustain. Chem. Eng. 2026, 14, 13517−13532

study, 2020 levelized costs of different HVC production technologies are compared in Figure S1 to better understand the economic feasibility of low-emission technology adoptions.

Details of the designed scenarios are described in Table 1. For scenarios with no carbon constraint (NCC), it is assumed that the domestic HVC sector adopts the least-cost technologies without strong carbon mitigation commitments. For scenarios with a net-zero emissions (NZE) target, the industry must reach net-zero, considering decarbonizing upstream emissions from oil and gas refining by 2050. The net-zero emissions (NZE) target in this study is defined as a 100% reduction in GHG emissions relative to 2020 levels by 2050. Crucially, the system boundary for this constraint extends beyond direct facility emissions to include indirect emissions from electricity and upstream fugitive emissions from the extraction and refining of fossil feedstocks (ethane, propane, and naphtha). NZE variant scenarios aim to explore how the HVC sector can be impacted by technology enhancement in bioenergy, clean hydrogen, and circular economy development. NCC variant scenarios focus on examining whether policy interventions, including carbon pricing and tax incentives under the recent U.S. Inflation Reduction Act (IRA), could accelerate the decarbonization transition for the HVC sector. In addition to the scenario analysis for potential net-zero pathways under plausible conditions, this study explores the impacts of system and technology variations on the technology transitions given different system perspectives and uncertainties about future technology development (see Table 1).

In all scenarios, this study adopts a U.S. domestic HVC production growth rate and projects the future demand by 2050 based on historical data from the U.S. Energy Information Administration (EIA)[26,27] and the Independent Commodity Intelligence Services (ICIS) database,[28] details of which can be found in Table S3. From a baseline of 41.4 million metric tons HVC in 2020 (comprising 34.7 Mt ethylene, 4.6 Mt propylene, and 2.2 Mt BTX), total demand is projected to reach 59.8 million metric tons by 2050. This represents an average annual growth rate of approximately 1.2% across the sector. As shown in Figure 3, the HVC demand expansion would result in a 24% increase in annual greenhouse gas emissions relative to 2020 levels in the absence of mitigation efforts. This study considers future changes in fuel and feedstock prices, production technology emissions intensities, and equipment capital investments. The U.S. EIA's Annual Energy Outlook 2023[29] reference case and low zero-carbon technology cost case were used for energy price projections in the NCC and NZE scenarios, respectively. The time horizon is set from 2020 to 2050, and the discount rate is assumed to be constant as 5%.[30]

The HVC production projections for 2050 focus primarily on HVCs produced in the chemical sector rather than coproducts produced in the oil and gas refinery sector. Therefore, this study focuses on how today's HVCs produced in the petrochemical sector could be transitioned to near-zero carbon performance levels.

In all NZE scenarios, the carbon mitigation plan including upstream emissions is constrained to reduce 25% of the 2020 emission level by 2030 and it will reach net zero by 2050, which is in line with the mitigation goals proposed in the International Energy Agency (IEA) Net Zero Emissions by 2050 scenario.[25]

This model considers constraints on the maximum available amount of blue hydrogen, bioethanol, and sorted plastics. Blue hydrogen availability is based on the potential hydrogen production from natural gas reforming for other uses except for uses in the ammonia, methanol (35%), and refinery sectors (55%) in the U.S.[35] The projection of hydrogen production is estimated based on data from the U.S. EIA.[36] In the U.S., bioethanol is produced from a fermentation process using corn starch as feedstock and the annual production capacity is 14 billion gallons.[37] This study assumes that the availability of bioethanol used as feedstock for ethylene production is the amount of annual export plus end stock and the annual growth rate of available bioethanol is 0.1 billion gallons. The availability of sorted plastics is estimated based on the historical data of annual municipal solid waste generation and the recycling rates of plastics.[38] The mixed sorted plastics mainly include HDPE, LDPE, PP, PET, PS, and PVC and exclude plastic waste from construction, textiles, and other non-MSW sectors. This study assumes that recycling rates of mixed and pure sorted plastics can be increased up to 0.5% annually in all scenarios except for NZE-HighCE scenario. This estimated upper bound of recycling rate growth is based on the average value between U.S. historical data on the recycling rate[38] and the global increasing recycling rate evaluated by Geyer et. al.[39] In addition, the maximum portion of these mixed sorted plastics that can be reprocessed by mechanical recycling is constrained at 80%[40] considering the quality and contamination of collected plastic waste. Chemical recycling is applicable for reprocessing the remaining 20% of mixed sorted plastics. Detailed data on resource availability can be found in Table S4.

This study investigated two alternative pathways for decarbonizing bioethanol production: CCS and utilization of renewable natural gas (RNG) from biogas. The result indicated that bioethanol equipped with CCS is more economically competitive than bioethanol fueled by RNG. Therefore, this study only compares results between NZE-BECCS and other scenarios. The model considers blue and green hydrogen as an energy source imported from upstream processes with specific costs. Therefore, capital investments in clean hydrogen infrastructure are not included in the results of system costs. Across all scenarios, a 0.1% annual capacity expansion is applied to mechanical recycling facilities, accounting for the technology's cost-competitiveness as an alternative route for domestic HVC supply. The IRA 45Z tax credit for incentivizing clean fuel production, such as bioethanol, is not investigated in the model since it is only available from 2025 to 2027. The detailed tax credits for each qualified low-emission technology pathway under 45Q and 45 V are given in Supplementary Table S10, including detailed scenario input comparisons.

RESULTS

Technology Transitions for Net-Zero

Figure 2 shows the production share by technology over the time horizon under the NCC, core NZE, and NZE variant scenarios. In the NCC scenario, ethane cracking and propane dehydrogenation (PDH) are the dominant technologies by 2050 for producing ethylene and propylene, respectively. Without the carbon mitigation constraint, the ethylene production of recycling processes (mechanical recycling, pyrolysis, and dissolution) only contributes to 17% of the total demand. However, propylene and BTX produced by recycling processes account for 41 and 83%, respectively. The recycling processes (e.g., mechanical recycling for polyethylene terephthalate (PET) and dissolution for low-density polyethylene (LDPE) and polypropylene (PP)) have lower HVC production costs compared to conventional technologies (e.g., ethane cracking and propane dehydrogenation). The HVCs attributed to mechanical and dissolution recycling are estimated as avoided virgin materials displaced using recycled plastics as feedstock. Consequently, all outputs from these recycling processes are treated as demand reduction measures for the primary chemical sector rather than as direct chemical production.

In the core NZE scenario, nearly 50% of ethylene production from existing ethane cracking needs to be retrofitted with CCS technologies by 2035 to meet the carbon mitigation goal. By 2050, CCS-equipped ethane cracking produces the largest share (65%) of ethylene production, followed by electrified ethane cracking (EEC) with byproduct upgrades. Water electrolysis-based methanol to olefins (WE-MTO) plays a significant role in achieving the net-zero target for HVCs since it is the only negative-emission technology deployed under the core NZE scenario. The contribution from recycling processes to the total

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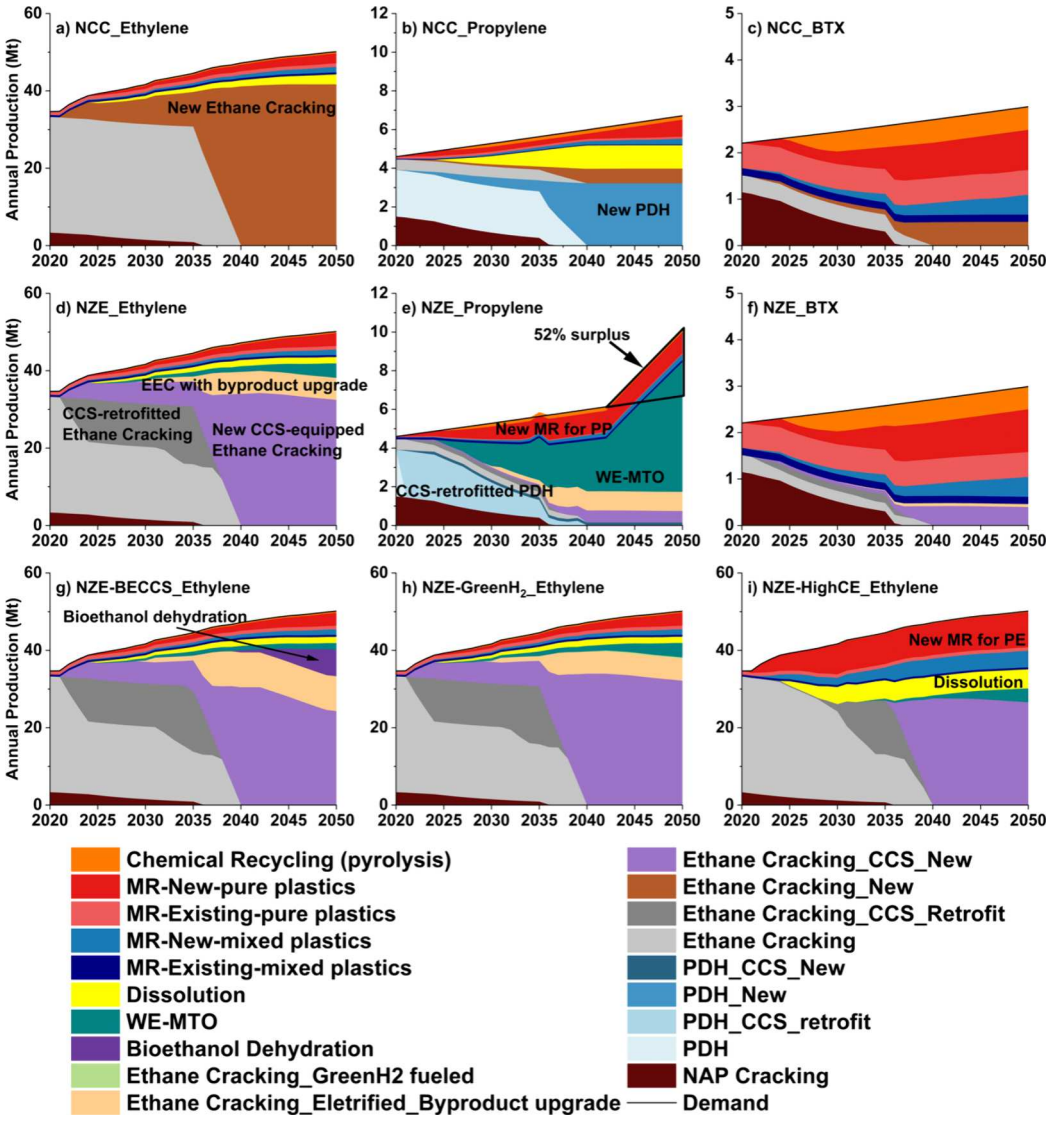

Figure 2. Production share of technology for HVC production under the (a–c) NCC, (d–f) NZE, and (g–i) ethylene production for NZE variant scenarios. See Figure S2 for HVC production share of all NZE variant scenarios. (For mechanical recycling and dissolution technologies using pure sorted plastics as feedstock, ethylene is obtained from HDPE and LDPE, propylene is obtained from PP, and ethylene and BTX are obtained from PET. Under the core NZE and NZE variant scenarios, 86% of chemical recycling production capacity is equipped with CCS technology and the remaining capacity is electrified pyrolysis).

ethylene demand decreases slightly compared to the NCC scenario from 17 to 16%. The major change in the recycling processes is the shift from dissolution to mechanical recycling due to the higher emission factor of the dissolution process. HVC production from mechanical and chemical recycling technologies can be seen as a demand reduction for raw materials used in polymers and other applications.

It should be noted that propylene production has a 52% supply surplus under the core NZE scenario. This surplus of propylene supply is the consequence of WE-MTO deployment, which mainly aims to decarbonize the carbon emissions of ethylene production. There are two aspects to consider regarding this surplus. First, the HVC industry might not simply adopt the expensive WE-MTO technology due to this imbalance between propylene supply and demand and the extremely high investment costs. On the other hand, this surplus of propylene production might offset a shortage in the supply from the refinery sector when the fossil-fuel refining processes phase out in the future. The BTX manufacturing processes in the core NZE scenario are similar to the transition in the NCC scenario, except for the shift from conventional ethane cracking to CCS-equipped ethane cracking and EEC with a byproduct upgrade process. In the core NZE scenario, all recycled HDPE and LDPE will be used as secondary materials in the mechanical recycling and dissolution processes for ethylene production due to the low cost of sorted plastic bales. The utilization rates of mixed plastic waste, pure sorted PP, and PET of the available stock are 90, 50, and 79%, respectively.

As it is mentioned that the core NZE scenario will have a large propylene supply surplus from WE-MTO when decarbonizing the entire HVC sector, this study performs a sensitivity analysis associated with an adjustment of the yield ratio of ethylene to propylene from 0.6 to 1.3.[22] The results shown in Figure S3 indicate that the HVC sector could have a lower

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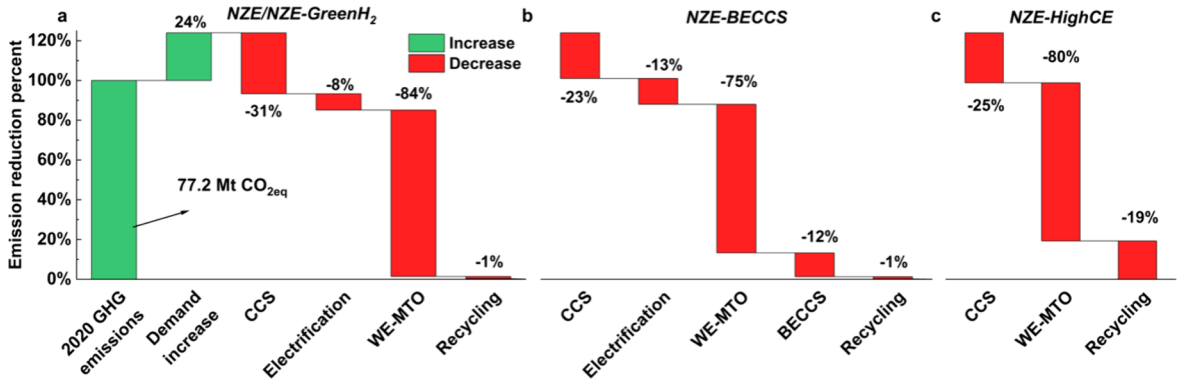

Figure 3. Contributions of adopted mitigation levers to the net-zero emissions in the (a) NZE/NZE-GreenH$_2$; (b) NZE-BECCS; and (c) NZE-HighCE scenarios. The green bar indicates the total GHG emissions in 2050 under NCC scenario. Red bars are mitigation steps to net zero emissions by different mitigation levers.

propylene surplus of 28% with a higher yield ratio of ethylene to propylene in the WE-MTO process in the core NZE scenario.

In the NZE-BECCS, CCS-equipped bioethanol dehydration (BD) is the key negative-emission technology for decarbonizing ethylene production, and it is economically competitive with WE-MTO. Since a large portion of WE-MTO is replaced by CCS-equipped BD with more captured and sequestered CO_2, ethylene production can be produced more by the conventional ethane cracking process compared to the production share in the core NZE scenario. Moreover, no more surplus of propylene is supplied from WE-MTO in this case. Therefore, promoting the adoption of BD with CCS technologies could be a viable way to decarbonize the HVC industry by 2050. This study considers the maximum availability of corn bioethanol production as feedstock for ethylene based on the current export level, with an annual growth rate of 0.1 billion gallons.

When the production cost of green hydrogen is reduced to US$1/kg, aligning with the U.S. Department of Energy's clean energy strategies[41] in the NZE-GreenH$_2$ scenario, green H$_2$-fueled ethane cracking will be more cost-effective in 2040 compared to CCS-equipped ethane cracking for ethylene production. It starts replacing the CCS-equipped ethane cracking capacity slowly with less than 1% of the total ethylene production supply. WE-MTO is still required to achieve the net-zero target. Therefore, green hydrogen might not be significant for the HVC industry to achieve the net-zero emission target by 2050 with a cost of US$1/kg. Given the uncertainty in the future green hydrogen production cost from water electrolysis powered by renewable electricity, this study conducted a sensitivity analysis and found that a breakeven point of US$0.9/kg green hydrogen enables green hydrogen-fueled ethane cracking to be economically competitive with other technology routes. More details can be found in Figure S4. However, it is still challenging for the industry to reduce the green hydrogen cost from $5–7/kg to $1/kg, considering high costs of electrolyzers, renewable electricity prices, and the cost competitiveness of blue hydrogen.[42]

In the NZE-HighCE scenario, this study assumes the recycling rate of plastics will be 50% during 2030–2050 based on the EPA's National Recycling Strategy.[3] Although ethylene is not produced from mechanical recycling processes, 40% of ethylene demand for PE and PET will be fulfilled by recycling processes by 2050. Under a high circular economy of plastics, no new CCS-equipped ethane cracking plants are required until 2035 and no adoption of EES with byproduct upgrade is needed by 2050 to achieve the carbon mitigation target. This is attributed to the lower emissions from the upstream processes of recycled plastics compared to the fossil fuel-based feedstocks. However, WE-MTO still has a similar production share of ethylene (7%) in this scenario and that leads to a total 64% supply surplus of propylene. Similar to the core NZE scenario, 100% of available recycled HDPE and LDPE will be used for ethylene production. The utilization of mixed plastic waste and sorted PP increases by 140% and 165%, respectively, compared to the core NZE scenario by 2050. However, the use of recycled PET will be reduced by 40% compared to the core NZE scenario, given the high cost of PET bales, and the ethylene and BTX demand can be supplied by mechanical recycling from more available sorted PE and mixed plastic wastes.

Figure 3 indicates the contributions of mitigation levers adopted by different NZE scenarios to the net-zero emission goal for the HVC industry. Across all NZE scenarios, WE-MTO has the largest contribution to reducing the total emissions, which is attributed to the captured carbon used to synthesize methanol for the MTO process. The deployment of CCS technology for ethane cracking and PDH can reduce the total emissions by 19–25% under various scenarios. Electrified ethane cracking is the major electrification lever with a contribution to 7–11% emission reduction. In the NZE-BECCS scenario, bioethanol dehydration equipped with CCS can reduce 10% of the total emissions and the contribution of WE-MTO decreases to 60%. Compared to other NZE scenarios, the recycling technologies in the NZE-HighCE scenario have a larger contribution (16%) to the emission reduction. Since less than 1% of the ethylene supply is produced by green hydrogen-fueled ethane cracking, the total contribution landscape of low-emission technologies in the NZE-GreenH2 is similar to the core NZE scenario.

Technology Transitions under Policy Interventions

Results of technology shares in 2050 under the NCC-CP and NCC-IRA scenarios are shown in terms of propylene production in Figures 4 and 5, respectively.

In the NCC-CP scenario, EEC with byproduct upgrade technology becomes more cost-effective than the conventional

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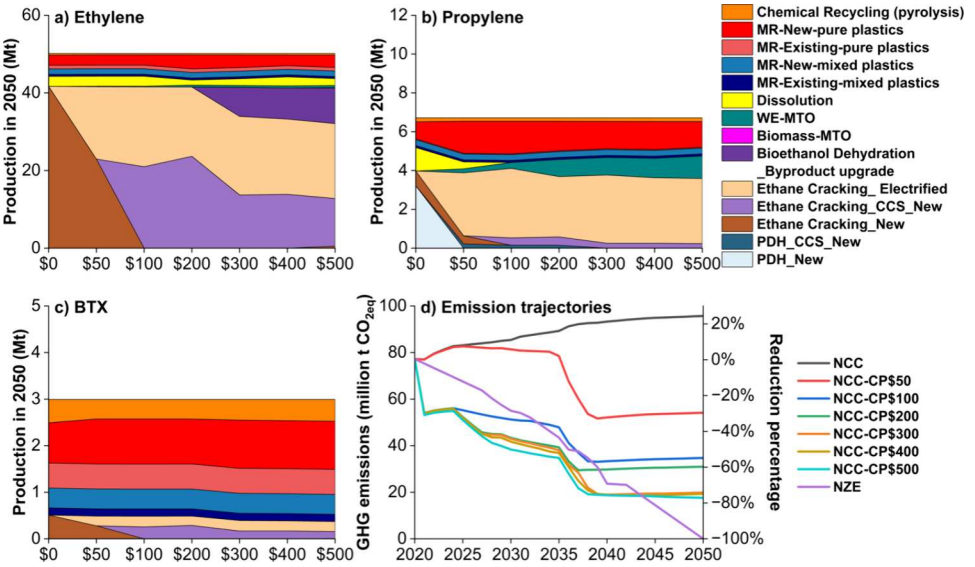

Figure 4. Production share of technology for HVC products in 2050 relative to a variety of carbon prices (US$0–500/t CO_{2eq}) for (a) Ethylene, (b) Propylene, (c) BTX, and (d) emission trajectory under various carbon prices between 2020 and 2050 (left Y axis: total GHG emissions; right Y axis: reduction percentage compared to the level in 2020).

ethane cracking under a carbon price of US$50/t CO_{2eq}, where the EEC with byproduct upgrade technology for HVCs starts to be deployed. The CCS-equipped ethane cracking route becomes more economically competitive than the EEC with byproduct upgrade technology under a carbon price of US$100/t CO_{2eq}. With a carbon price increase of up to US$200/t CO_{2eq}, mechanical recycling for pure sorted plastics turns out to be more cost-effective than the dissolution process. Moreover, the HVC industry is likely to adopt WE-MTO technology to produce ethylene and propylene with carbon credits from the negative process emissions. Therefore, less ethylene and propylene are produced from the EEC with the byproduct upgrade process as more propylene is generated from the WTO process. When the carbon price is between US$300–500/t CO_{2eq}, ethylene produced by bioethanol dehydration can be economically viable and replace a portion of the technology share of CCS-equipped ethane cracking. However, within a plausible range of carbon prices, i.e., from $100 to 500/metric ton, the HVC industry can only reduce the total GHG emissions by 60–77% compared to the level in 2020 (see Figure 4d).

Given the current 45Q tax credits for CCS technology deployment, the existing tax credit window is not likely to be effective in triggering the decarbonization technology transition for the HVC sector. However, with an extension of 45Q, ethane cracking, PDH and chemical recycling processes can become economically beneficial with CCS retrofits, and the total emissions by 2050 can be reduced by 23%. With the current 45 V tax credits applied for clean hydrogen production, the propylene production cost of WE-MTO becomes cheaper than the costs of conventional PDH process technology. Furthermore, WE-MTO can replace a large portion of the PDH and dissolution for propylene production under an extension of the 45 V. However, based on the emission trajectory result in Figure 5i, the current or extended IRA implementations are unlikely to enable the HVC industry to reach a net-zero emission target without the carbon mitigation constraint.

Tradeoffs in Emissions, Energy Consumption, and System Costs

Cumulative Emissions. Graphs in the first column in Figure 6 show the annual emissions and net cumulative emissions by 2050 under the NCC, core NZE, and NZE variant scenarios. Compared to the annual emissions under the NCC scenario, the NZE scenario can reduce the upstream and direct emissions by 68% in 2050. The remaining emissions mainly result from the upstream ethane refining process, and those remaining emissions can be balanced by carbon removal via the WE-MTO process. The NZE-GreenH2 scenario has the largest annual positive emissions in 2050 and cumulative emissions. Among the NZE variant scenarios, NZE-HighCE has the least emissions from upstream and direct processes, which is attributed to the high recycled plastic use for HVC production. However, the cumulative emissions of this scenario are the highest. In the NZE-BECCS scenario, negative emissions from bioethanol dehydration contribute 46% of the total negative CO_2, and the carbon removal from bioethanol dehydration allows more positive emissions from upstream and direct emissions under the net-zero emission constraint for the HVC sector. NZE variant scenarios have close net cumulative emissions with a range of 1.27–1.29 (an average 53% reduction compared to NCC) billion metric tons CO_{2eq} by 2050 and most cumulative emissions are emitted by upstream extraction of feedstock and fuels.

Energy Consumption. Energy consumption includes feedstock, fuel, and electricity used for HVC production technologies. Feedstock inputs include raw materials extracted from fossil fuels (naphtha, ethane, and propane), recycled plastics, and bio-based materials. Energy sources for processing heating for HVC production are natural gas, electricity, and hydrogen. NZE-HighCE has the least amount of total energy demand among the NZE variant scenarios and requires 0.11 exajoules (EJ) less than the NCC scenario. This is because recycled plastics are used to substitute fossil fuels as feedstock for HVC

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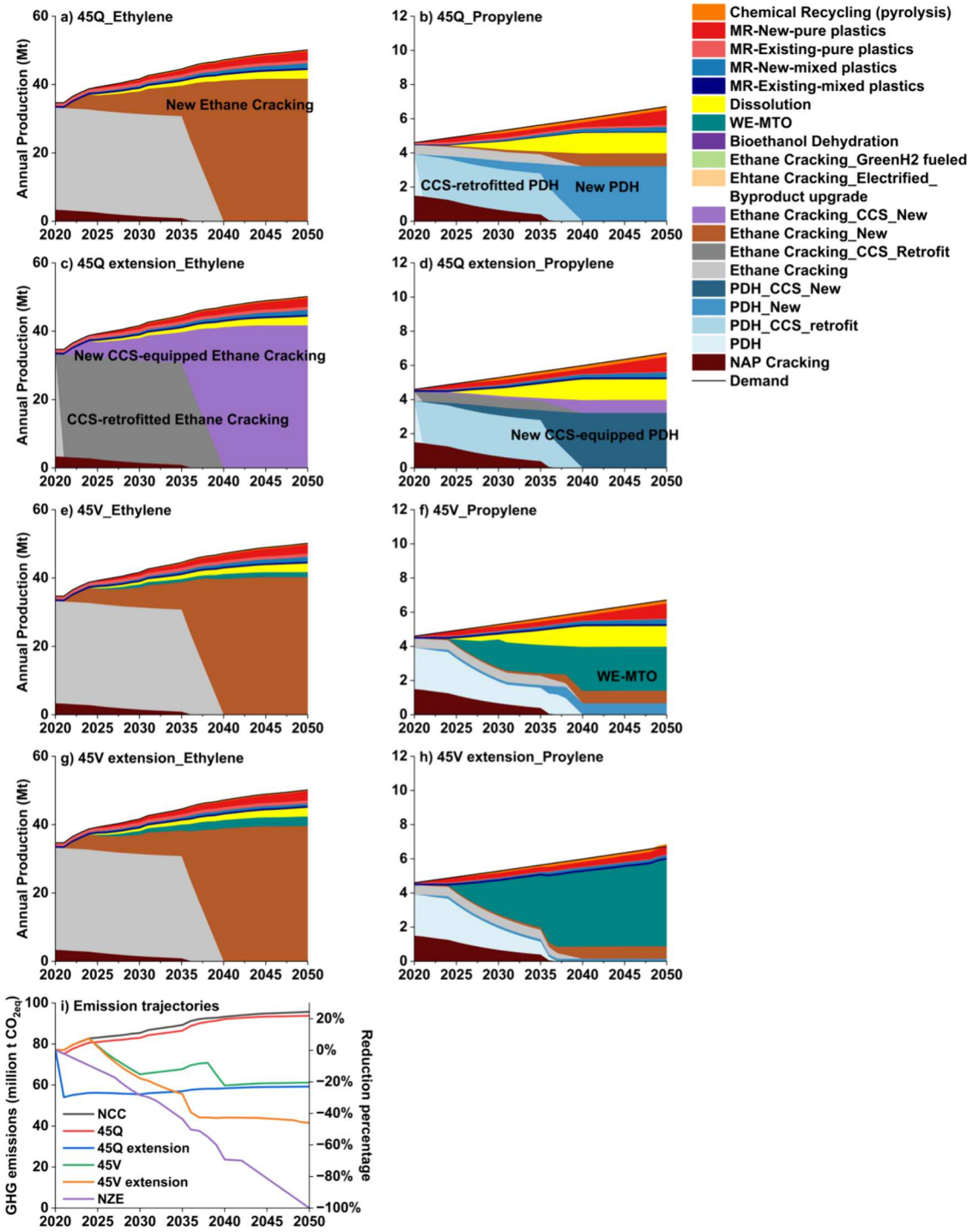

Figure 5. Production share of technology for ethylene and propylene demands under (a, b) NCC-45Q, (c, d) NCC-45Q extension, (e, f) NCC-45 V, and (g, h) NCC-45 V extension scenarios and (i) emissions trajectories of NCC, NZE, and all NCC IRA scenarios (left *Y* axis: total GHG emissions; right *Y* axis: reduction percentage compared to the level in 2020). See Figure S5 for HVC production share of all NCC variant scenarios. The current 45 V and 45Q tax credits are eligible for facilities that are constructed before 2033. The extensions for 45 V and 45Q are assumed to be available until 2050.

production. A significant amount of renewable electricity (0.7–1.2 EJ per year, or 0.2–0.3 million GWh per year) is needed for the HVC sector to achieve a net-zero target in 2050. However, the demand for renewable electricity could be reduced by enhancing the deployment of BECCS and plastic recycling, as assumed in the NZE variant scenarios. In the NZE-HighCE scenario, more recycled plastics can be reprocessed for HVCs, and it reduces the ethane consumption by 32% compared to the core NZE scenario.

By 2050, the HVC sector will likely still rely on ethane production from oil and gas refineries as a cost-effective feedstock for HVC production. This result implies that the chemical

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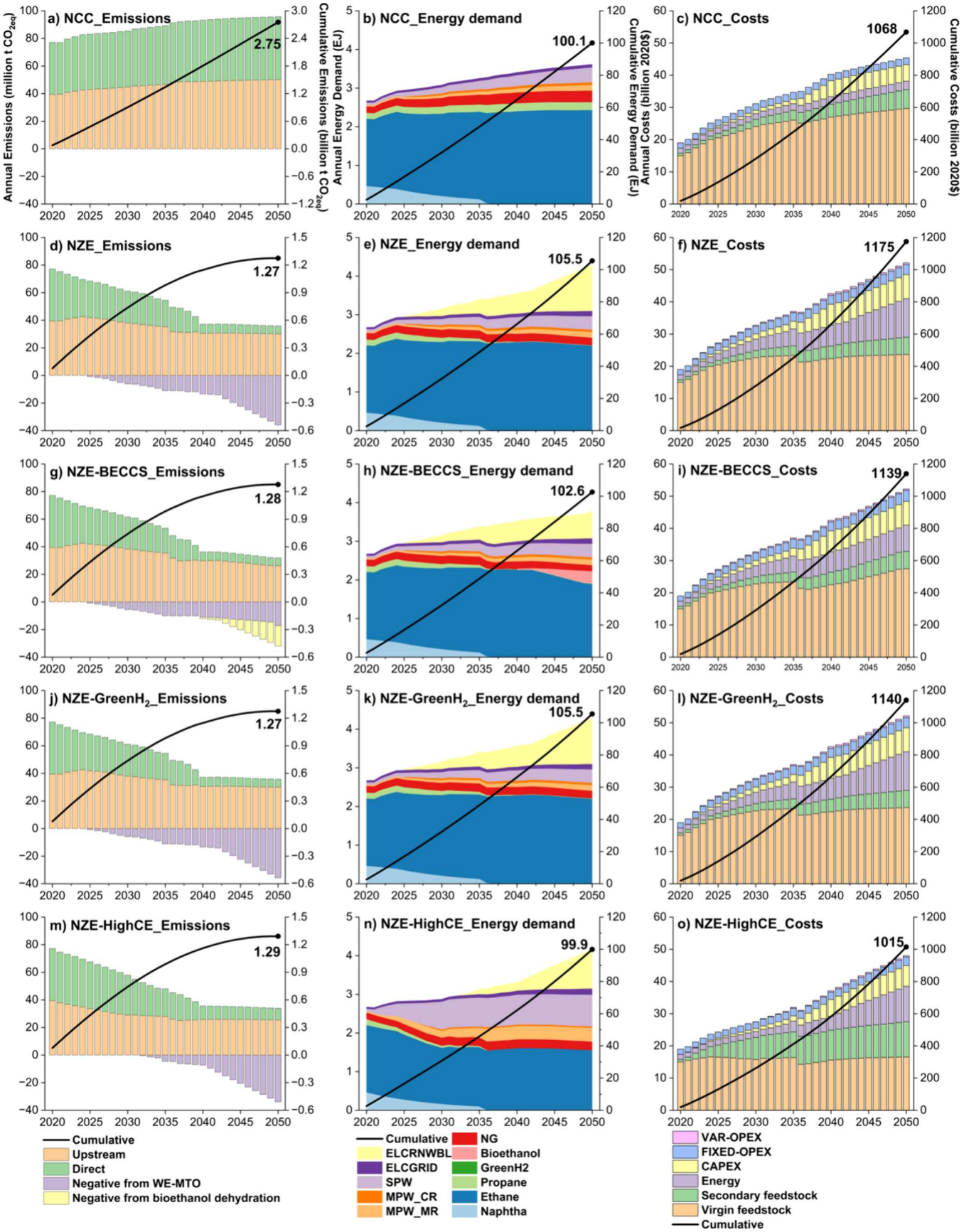

Figure 6. Annual (left *y* axis) and cumulative (right *y* axis) emissions, energy demand, and system costs under (a–c) NCC, (d–f) NZE, and (g–o) NZE variant scenarios. (Cumulative values by 2050 of emissions, energy demand, and system costs are labeled with numbers).

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industry is expected to become one of the largest drivers of oil and gas consumption in the future, while fossil fuels might be phased out from other sectors.[6] Moreover, it might affect the entire technology landscape for the HVC sector to reach net zero if the oil and gas refinery sector can reduce the emissions of ethane and propane production. In the U.S., the majority of propane is produced as a byproduct of natural gas processing and the emission factor of propane production is assumed to be 0.083t CO_{2eq}/GJ.[43,44] However, the emissions of propane from crude oil refining are estimated to be 0.012t CO_{2eq}/GJ.[44] If emissions of propane production from natural gas extraction can be reduced or substituted with propane from oil refineries, less effort might be needed to deeply decarbonize the HVC and other chemical sectors.

System Costs. This study compares the system costs between various scenarios in terms of feedstock cost of raw and secondary materials, energy cost, variable and fixed operation costs (VAR-OPEX and FIXED-OPEX), and capital expenditures (CAPEX). Graphs in the third column in Figure 6 show annual system costs in 2050 and cumulative system costs by 2050 under the NCC, core NZE, and NZE variant scenarios. Without the emission constraint, the annual system costs for the HVC industry will increase to US$45.4 billion in 2050, which is more than two-fold the costs in 2020. To achieve the net-zero emission target, annual system costs will further increase by 24% compared to the costs in the NCC scenario. In the core NZE scenario, annual raw material cost will decrease in 2050 with a huge increase in energy cost due to the intensive renewable electricity consumption (76% of the total energy cost) for the WE-MTO process. Among the three NZE variant scenarios, NZE-HighCE has the lowest annual system costs resulting from lower feedstock costs of recycled plastics. In the NZE-GreenH_2 scenario, the deployment of green hydrogen-fueled ethane cracking has a negligible change in the total system costs. In the NZE-HighCE scenario, the cost of recycled plastics for mechanical recycling doubles the secondary material cost in the core NZE scenario, while the raw material cost of ethane reduces by 30%. The raw material cost is the major cost that accounts for 49–71% of the cumulative system cost by 2050 among the considered scenarios. The cumulative CAPEX for the NZE variant scenarios is around 40% higher than the CAPEX in the NCC, except for the NZE-HighCE scenario (only a 10% increase). However, this study indicated that the decarbonization scenarios have a cost parity with the non-carbon constraint case. Furthermore, the NZE-HighCE has the lowest cumulative system costs among all scenarios. Therefore, achieving a high circular economy goal for plastic waste not only reduces the environmental impacts of plastic waste management but also provides a more cost-effective way for a net-zero emission HVC industry. Detailed results of cumulative emissions, energy demand, and system costs are provided in Table S11.

Uncertainty in Energy Prices. Energy prices are identified as a key factor that drives the technological transition patterns and come with large uncertainties in their projections. This study conducts an uncertainty analysis to explore the effect of low and high energy price projections on technology transitions to NZE associated with changes in emissions, energy demand, and system costs. Low and high energy price projections of energy sources are based on energy price ranges estimated by the AEO Outlook 2023 cases as given in Table S12. With uncertain future energy prices, the major change in the NZE technology landscape is the shift from electrified ethane cracking to ethane cracking equipped with CCS technologies under a low energy price condition, particularly when oil and gas prices are low, and vice versa. However, this change has limited impacts on the overall technology deployment structure for NZE. Meanwhile, changes in cumulative emissions and energy demand are subtle as shown in Figure 7a,b. Cumulative system cost has considerable changes caused by the uncertainty in energy prices that affect the costs of energy consumption (error bars indicate annual system cost ranges). Cumulative system cost decreases and increases by 9% by 2050 under a low and high energy price case, respectively, as shown in Figure 7c.

Influences of System Boundary Variations. First, an NZE scenario that excludes upstream emissions (NZE-Direct) is considered to represent a possible case in which the HVC sector has no responsibility for the upstream emissions from petrochemical feedstock refining. Under this exclusion, the total system emissions will reduce to 3.8 million metric tons in the reference year of 2020. Figures 8d–f show the technology transitions under NZE-Direct scenario. The major difference between the core NZE and NZE-Direct is the technology transition from the CCS-equipped ethane cracking to conventional ethane cracking and EEC with byproduct upgrade since upstream emissions are excluded. In addition, a significant decrease occurs in the technology share of WE-MTO resulting from less system emissions to sequestrate. These results show how important a comprehensive carbon emissions boundary can be for identifying needed net-zero technology transitions.

Second, this study investigates the ways to deeply decarbonize each HVC product separately (NZE-Separate) instead of as an integrated system. Since ethylene accounts for almost 85% of total HVCs and propylene and BTX are often produced as byproducts in ethane cracking, the priority is to decarbonize the emissions from ethylene production. Figure 8g indicates that the major decarbonization technology for ethylene production is CCS-equipped ethane cracking when ethylene production is deep decarbonized independently. The deployment of WE-MTO is projected to be between 2038 and 2050. Similarly, Figure 8h. shows that propane dehydrogenation emerges as the predominant technology in conjunction with WE-MTO and the breakdown of sorted PP plastics under the independent net-zero scenario. For decarbonizing BTX production separately, chemical recycling via pyrolysis and electrified naphtha cracking offers cost-effective pathways. Additionally, a significant portion of BTX demand can be satisfied through mechanical recycling and dissolution from sorted PET plastics.

Third, a sensitivity analysis for various carbon constraints (VCC) is conducted to examine whether lowering the carbon constraint can avoid large investments in expensive technologies (e.g., WE-MTO) for the HVC industry. Figure 8j. shows that the ethylene production share of WE-MTO reduces to 1.3% while there is no propylene surplus under a mild carbon mitigation target of 30%. Although WE-MTO is a costly technology for HVCs, it is indispensable for the HVC industry to reach the net-zero target. Further technological improvements are needed to reduce the high capital investment and operational costs for facilitating the deployment of this technology.

Finally, this study simulates decarbonization pathways for the HVC sector with postponed transition starting years

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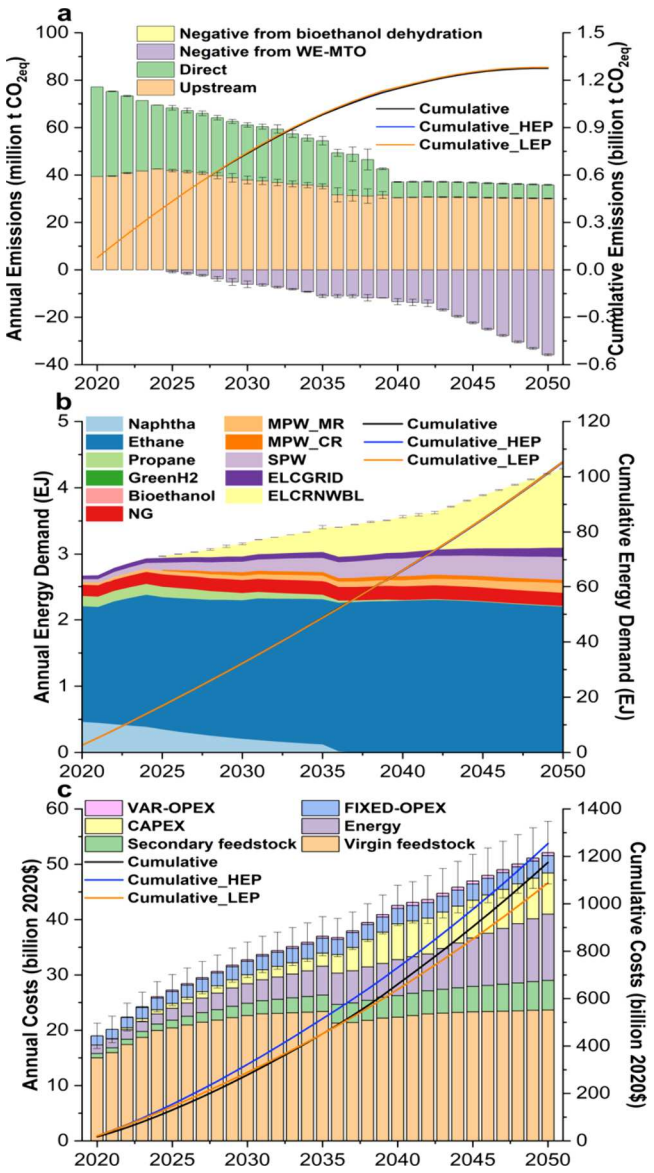

Figure 7. NZE scenario's annual (left *y* axis) and cumulative (right *y* axis) (a) emissions, (b) energy demand, and (c) system costs under low (LEP) and high (HEP) energy prices.

(NZE-PTSY) to evaluate the consequences when the system faces a delayed advanced technology maturity situation. Figure 8k. shows the emission trajectories of NZE scenarios with different starting years of decarbonization. Given a later transition starting point, the steeper required emission reduction trajectory is observed. This results in larger investments in the WE-MTO technology process for HVCs to achieve the net-zero emission goal associated with a larger propylene surplus. However, the emission reaches the peak point in 2024 although all cases have a later starting year of decarbonization. This result indicates that the HVC should start decarbonizing the HVC industry no later than 2025 under current and emerging low-emission technology landscapes to reach the net-zero emission goal by 2050. Otherwise, the HVC sector might not achieve the net-zero emission target by 2050 or require higher levels of investments to speed up the decarbonization pathway.

DISCUSSION

This study demonstrates how the U.S. HVC industry can transform into a net-zero system through the deployment of least-cost low or negative-emission technologies under various plausible technical, economic, and political conditions. In addition, scenario analyses of policy interventions examine what extent of carbon mitigation can be achieved by the implementation of IRA tax credits and carbon prices.

The HVC sector can achieve the net-zero emissions goal through extensive CCS and electrification for the ethane cracking process associated with WE-MTO deployment and recycling technologies for sorted plastics. This deep decarbonization pathway will need very large investments in the expansion of renewable electricity generation capacity dedicated to the HVC sector; for example, the demand for renewable electricity in the core NZE scenario is estimated to be 1.2 EJ in 2050, which is almost equal to the total U.S. generation from solar and wind sources in 2020. It should be noted that the WE-MTO technology might not be deployed in practice for the HVC industry due to extremely high investment costs and renewable electricity costs. However, it is essential for the industry to reach the net-zero goal and the decarbonization scenarios have a cost parity with the non-carbon constraint case. This study further tests another scenario and found that the deployment of WE-MTO will not be necessary when ethylene production is decarbonized separately with an 80% or lower carbon emission reduction.

The alternative pathway under NZE-BECCS has the least propylene supply surplus (6%) meanwhile reducing significant dependence on renewable electricity consumed in the WE-MTO route. However, the tradeoff of this pathway is higher cumulative system costs by higher feedstock purchases due to the deployment of CCS-equipped bioethanol dehydration. The carbon removal of bioethanol production can be further improved by switching natural gas to biogas for heating processes, but the entire bioethanol dehydration process for ethylene will be less cost-effective. Since bioethanol is currently used for transportation fuels, increasing demand on bioethanol for HVCs might require additional land use for growing corn and other secondary generations of energy crops, and lead to other environmental (e.g., indirect land-use change, eutrophication, and biodiversity loss) and economic (e.g., price fluctuation) concerns for bioeconomy development.

Although green hydrogen could be produced at a low cost, using green hydrogen as fuel for ethane cracking will likely not be as cost-effective compared with CCS-equipped ethane cracking in a long-term decarbonization pathway. The extent of deployment and utilization of green hydrogen as fuels for HVCs production highly depends on the cost of green hydrogen production. To generate green hydrogen with or less than US$1/kg in the near-term, incentives (e.g., IRA 45 V tax credits), renewable electricity price reduction, and technology improvements (e.g., conversion energy efficiency and large-scale development of water electrolysis) are needed to reduce the cost of green hydrogen production.[45]

A more circular economy that complies with the national recycling goal provides a large availability of recycled plastics as feedstock for HVCs through mechanical, dissolution, and chemical recycling processes. Reprocessing recycled plastics from recycling technologies for HVCs, especially for mechanical recycling, can significantly reduce upstream emissions and

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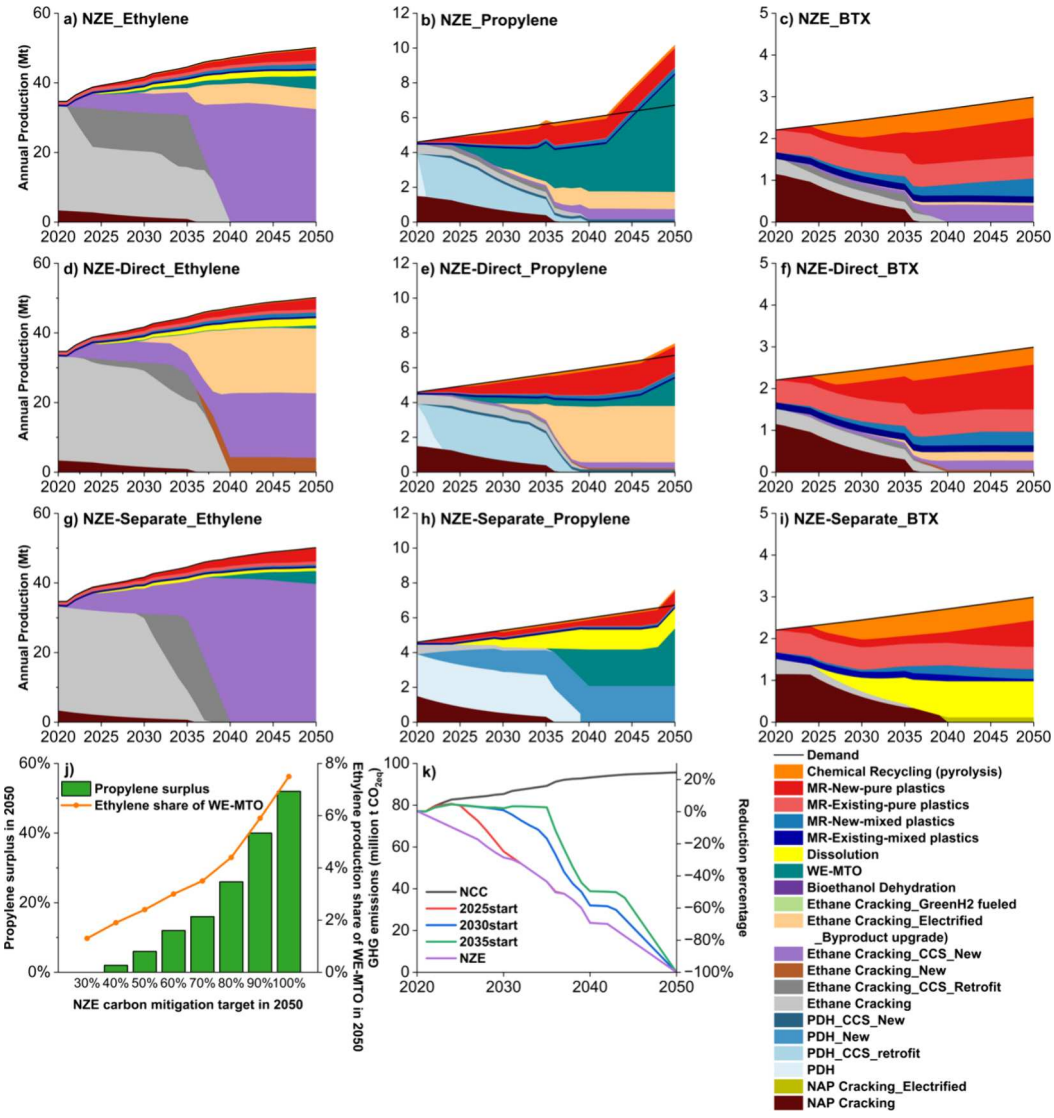

Figure 8. Production share of technology for HVC demands under (a–c) NZE, (d–f) NZE-Direct, and (g–i) NZE-Separate scenarios. (j) Propylene surplus and ethylene production share of WE-MTO under various carbon mitigation targets. (k) Emission trajectories of delayed timelines with decarbonization starting years of 2025, 2030, and 2035.

capital investments in low-carbon emission technologies, which leads to less cumulative energy consumption and system costs for decarbonizing the HVC industry. This study illustrated a scenario with an extremely high recycling rate of waste plastics to explore the maximum capability of emission savings from demand reductions in fossil fuel-based HVC feedstock. However, it is challenging for domestic waste management to increase the plastic recycling rate to 50% by 2030 with technical and economic obstacles in practical collection and sorting operations.[46] While other studies[8,47] suggest more conservative ranges for global or broad industrial recycling, the NZE-HighCE scenario illustrates the maximum potential for emission savings through aggressive demand reduction for fossil-fuel-based feedstock, even while acknowledging the significant technical and economic obstacles in practical collection and sorting operations that must be overcome to reach such levels. The technology transition pathway might differ than identified here if other advanced recycling technologies (e.g., enzymatic hydrolysis, glycolysis, methanolysis) are more cost-effective with high-quality recovered materials in the future. Compared to mechanical recycling, the CAPEX and high process emissions of chemical recycling via pyrolysis are the major disadvantages. Subsidies and incentives could reduce some burdens in capital investments in advanced recycling technologies for facilitating large-scale deployment of those technologies. The constraint assumptions on biomass resources and recyclable materials for mechanical and chemical recycling are made based on feedstock quality, technical maturity and competition with other applications.

These insights provided by this study are not only for potential net-zero pathways for the HVC sector but also for domestic plastics since HVCs are the major polymerization materials for plastics. Countries that have similar features with respect to energy portfolio and HVC manufacturing processes to the U.S. could find useful insights from potential alternative deep decarbonization pathways for HVCs to adjust their strategies

https://doi.org/10.1021/acssuschemeng.6c03082
ACS Sustain. Chem. Eng. 2026, 14, 13517−13532

to reach carbon mitigation targets. For example, countries like the Netherlands in Europe might adopt the technology transitions in the NZE-HighCE scenario corresponding to their ambitious circular economy target for plastics (100% circular for plastic production) by 2050. Countries like Brazil that have plentiful bioethanol production could expect a similar role of bioethanol dehydration in decarbonizing the HVC sector. Meanwhile, countries like China that have different HVC manufacturing technology routes and infrastructure may consider these pathways less transferrable to their contexts of decarbonizing the industry.

This research points to several limitations that can be explored in future work. First, this study did not explicitly model the upstream process technologies for feedstock production (e.g., ethane, propane, and natural gas). It is unclear when and how the oil and gas refinery would reduce the emissions from oil and gas processing operations, but such considerations might change the overall technology transitions and require less investment in the HVC sector. Second, although the model constrained the maximum availability of recovered plastics for mechanical recycling and other recycling technologies, all recovered plastics are assumed to be qualified for reprocessing to new plastics with the same quality as raw materials. It would be more robust to consider the acceptable rate of qualified recovered plastics and losses of final recycled plastics due to poor quality. Finally, this study only details the net-zero pathways on the supply side without considering the synergies with demand-side measures in HVC products. A net-zero HVC sector could be realized by making efforts to decarbonize production supply and decrease the future demand for HVC uses in plastics and other applications (e.g., single-use plastic ban, material substitution, etc.). Those measures could significantly lower the absolute demand for HVCs and such demand-side shifts would likely ease the pressure on the most expensive supply-side levers, like WE-MTO, and reduce the overall system cost of reaching net zero. Future work should explore the potential net-zero pathways under a demand reduction scenario for HVCs.

CONCLUSIONS

This study provides a robust, bottom-up framework for technology developers and policymakers to navigate the complex trade-offs of industrial decarbonization. Our analysis yields four primary conclusions: First, achieving a net-zero U.S. HVC sector by 2050 is technically feasible and, under optimized pathways, can achieve cost parity with non-carbon-constrained scenarios. Second, managing HVC production as an integrated system (accounting for ethylene, propylene, and BTX interdependencies) is significantly more cost-effective than attempting to decarbonize individual product streams in isolation. Third, while electrification and CCS are foundational, negative-emission technologies such as water electrolysis-based MTO and BECCS are indispensable for neutralizing residual upstream emissions. Finally, the high circular economy (NZE-HighCE) pathway emerges as the most cost-effective and resource-efficient strategy, mitigating 1.48 Gt CO_{2eq} while reducing the sector's reliance on capital-intensive technology and renewable electricity expansion. For decision-makers, these results emphasize that current policy frameworks, including the Inflation Reduction Act's 45Q and 45 V credits, require extensions or higher carbon pricing to bridge the gap toward a net-zero target. For academics, this work highlights the critical importance of a comprehensive carbon system boundary that includes upstream fugitive emissions to identify the true technology shifts required for deep decarbonization.

ASSOCIATED CONTENT

Data Availability Statement

The mathematical framework is documented in supplemental information. Any additional information required to reanalyze the data reported in this paper is available from the lead contact upon request.

Supporting Information

The Supporting Information is available free of charge at Https://pubs.acs.org/doi/10.1021/acssuschemeng.6c03082.

Techno-economic parameters for conventional and advanced HVC production technology pathways; projected technology capital expenditures (CAPEX) and energy source prices; historical and projected U.S. demand for ethylene, propylene, and BTX through 2050; assumed resource availability constraints for bioethanol, clean hydrogen, and plastic waste bales; inventory of announced commercial chemical recycling facilities; technical and economic assumptions for mechanical and chemical recycling; modeling parameters for U.S. federal tax credits under the Inflation Reduction Act (Sections 45Q and 45V); cumulative emissions, energy demand, and system cost results for all basic and variant scenarios; and uncertainty data regarding future energy price projections (PDF)

AUTHOR INFORMATION

Corresponding Author

Fanran Meng – *School of Chemical, Materials & Biological Engineering, University of Sheffield, Sheffield S1 3JD, United Kingdom*; orcid.org/0000-0002-9014-1231; Email: f.meng@sheffield.ac.uk. Tel.: +44(0) 114 2227510

Authors

Enze Jin – *Bren School of Environmental Science and Management, University of California, Santa Barbara, California 93117, United States*

Banafsheh Jabarivelisdeh – *Bren School of Environmental Science and Management, University of California, Santa Barbara, California 93117, United States*

Phillip Christopher – *Department of Chemical Engineering, University of California, Santa Barbara, California 93117, United States*; orcid.org/0000-0002-4898-5510

Eric Masanet – *Bren School of Environmental Science and Management, University of California, Santa Barbara, California 93117, United States; Department of Mechanical Engineering, University of California, Santa Barbara, California 93117, United States*

Complete contact information is available at: https://pubs.acs.org/doi/10.1021/acssuschemeng.6c03082

Author Contributions

Conceptualization: E.J., B.J., P.C., and E.M. Methodology, data curation, and formal analysis: E.J. and B.J. Writing—original draft: E.J. Visualization: E.J. and F.M. Writing—review &

https://doi.org/10.1021/acssuschemeng.6c03082
ACS Sustain. Chem. Eng. 2026, 14, 13517−13532

editing: F.M., P.C., and E.M. Funding acquisition: P.C. and E.M. Resources: P.C. and E.M. Supervision: P.C. and E.M.

Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGEMENTS

We acknowledge financial support from the C-THRU project: Carbon clarity in the global petrochemical supply chain (www.c-thru.org). Phillip Christopher and Eric Masanet acknowledge the Mellichamp Academic Initiative in Sustainability at UCSB for support. Fanran Meng gratefully acknowledges the support of the Royal Society ISPF—International Collaboration Awards (ICA\R1\231046).

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