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Integrated Assessment of the Leading Paths to Mitigate CO_2 Emissions from the Organic Chemical and Plastics Industry

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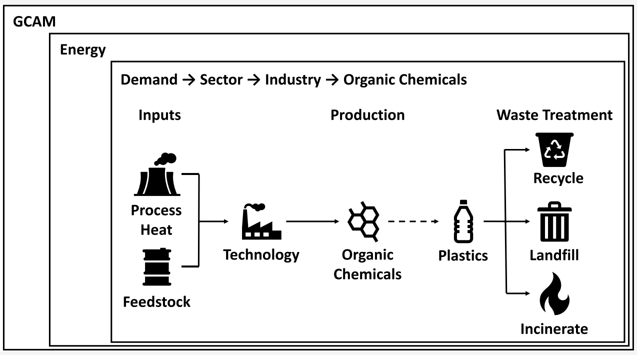

ABSTRACT: The chemical industry is a major and growing source of CO_2 emissions. Here, we extend the principal U.S.-based integrated assessment model, GCAM, to include a representation of steam cracking, the dominant process in the organic chemical industry today, and a suite of emerging decarbonization strategies, including catalytic cracking, lower-carbon process heat, and feedstock switching. We find that emerging catalytic production technologies only have a small impact on midcentury emissions mitigation. In contrast, process heat generation could achieve strong mitigation, reducing associated CO_2 emissions by ~76% by 2050. Process heat generation is diversified to include carbon capture and storage (CCS), hydrogen, and electrification. A sensitivity analysis reveals that our results for future net CO_2 emissions are most sensitive to the amount of CCS deployed globally. The system as defined cannot reach net-zero emissions if the share of incineration increases as projected without coupling incineration with CCS. Less organic chemicals are produced in a net-zero CO_2 future than those in a no-policy scenario. Mitigation of feedstock emissions relies heavily on biogenic carbon used as an alternative feedstock and waste treatment of plastics. The only scenario that delivers net-negative CO_2 emissions from the organic chemical sector (by 2070) combines greater use of biogenic feedstocks with a continued reliance on landfilling of waste plastic, versus recycling or incineration, which has trade-offs.

KEYWORDS: *plastics, chemicals, decarbonization, carbon capture, bioliquids, circular economy*

1. INTRODUCTION

Economy-wide efforts to reduce carbon emissions are needed to mitigate the worst impacts of climate change.[1] The chemicals manufacturing sector, including organic chemicals, is responsible for ~5% of global energy use and 6.5% of global greenhouse gas (GHG) emissions.[2,3] The chemical sector's share of global emissions is expected to increase as other sectors decarbonize and as demand for chemicals, which is closely linked to the demand for plastics, grows.[4−8] Pathways to decarbonize the sector are less clear than they are for many others, such as electricity generation and road-based passenger transportation. An analysis by the International Energy Agency (IEA) determined that ~70% of the energy used by the chemical sector is to produce a few chemicals: ammonia and organic chemicals (methanol, olefins, and aromatics).[4] The products and processes of the organic chemical industry are extremely diverse, and the products are subject to different uses and waste treatment options, implying there are no one-size-fits-all solutions for cutting the emissions in this sector. Accurate carbon accounting is also challenging because the organic chemical industry is deeply intertwined with fossil fuels, as both a feedstock and a source of energy. Unlike other industrial sectors such as iron and steel or aluminum, there is a major gap in the publicly available production data.[9] As a result, the integrated assessment models (IAMs) that provide guidance to decision makers about decarbonization pathways often rely on coarse representations of the sector.[10]

Recent reviews have identified crosscutting emissions mitigation options for the sector, including demand reduction, energy efficiency, fuel switching, recycling, bioproduction, and carbon capture and utilization or storage (CCUS).[8,11−14] To date, nonintegrated methods of analysis have lacked the ability to represent all of these pathways while also considering interactions with other sectors of the global economy. For example, several studies have concluded that the success of biobased products to reduce emissions depends on their fate at end of life.[15−17] The incineration of plastics derived from

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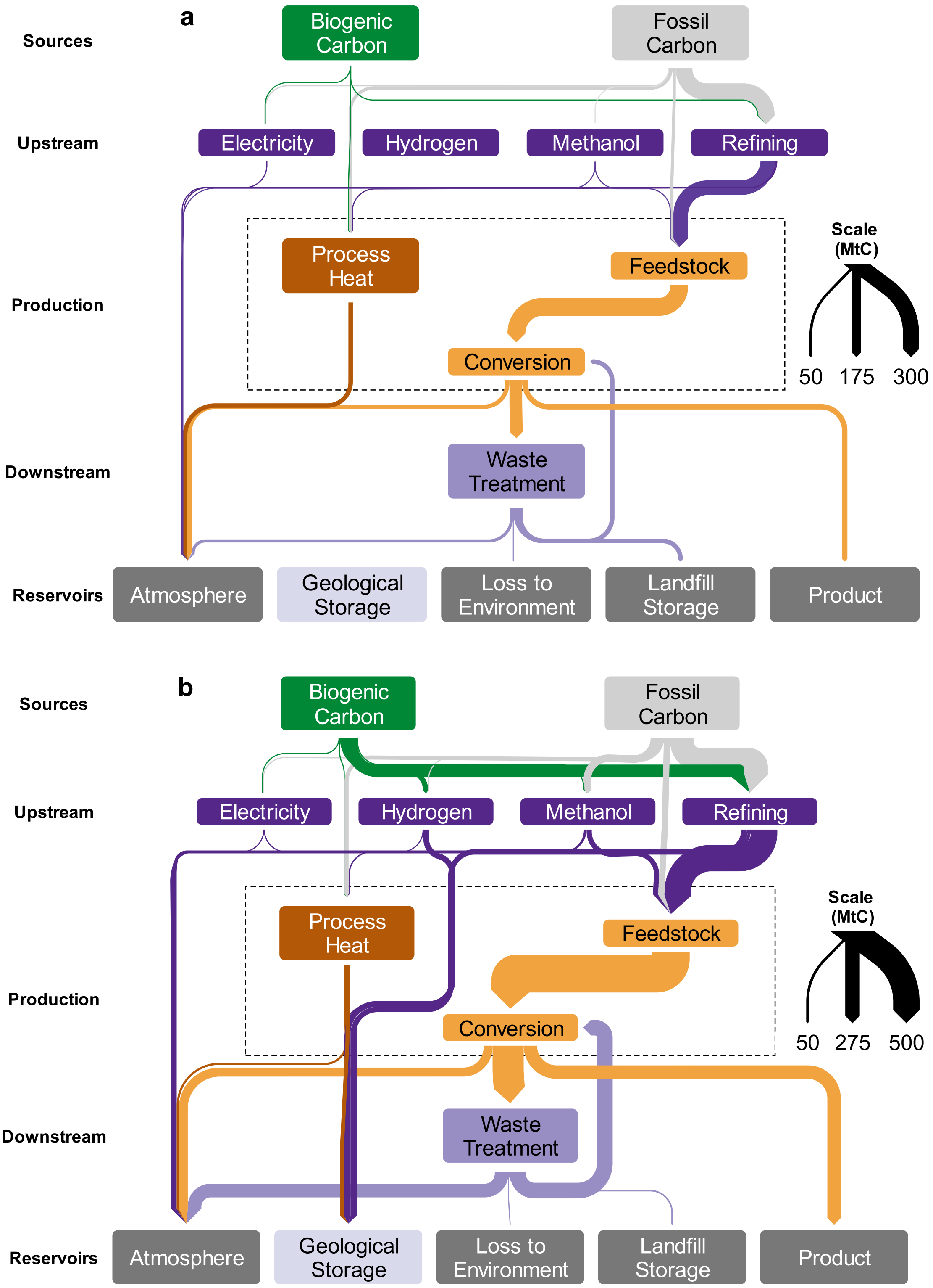

Figure 1. Flow of carbon in million metric tons (MtC) through the organic chemical sector in (a) 2015 and (b) a 2050 net-zero CO_2 policy scenario. We consider only hydrogen production for the generation of process heat and methanol production for feedstock for the organic chemical sector. The thickness of the lines indicates the relative volume, as indicated by the scale. An Excel workbook with the portrayed values is included with the data availability.

biomass has a similar carbon footprint to that of bioenergy without carbon capture and storage (CCS), at best achieving neutral (and more likely small positive) emissions. This is an improvement upon the use of fossil fuels but still imperfect in terms of achieving net-zero emissions. Further, electrification has the potential to reduce emissions in the chemical sector, although previous analyses have lacked an adequate representation of electrification's competition with CCS or clean hydrogen for providing process heat.[18−20] This highlights the need for detailed modeling to consider life cycle assessment (LCA), material flow analysis (MFA), and other energy and technological transitions when assessing the organic chemical sector. Even when studies have included a diverse representation of decarbonization pathways, they have often been limited in geographical scope or lacked interconnections and representations of other economic sectors. For instance, Sun et al. analyzed refinery sector emissions mitigation in the United States but did so in isolation from the remainder of the economy.[21] While these nonintegrated approaches have advanced our understanding of the potential for emissions mitigation in the organic chemical sector, there is still much to be gained from a simulation of all of these mitigation strategies in an economy-wide integrated fashion.

Other efforts to represent the chemicals sector in IAMs have produced important insights. Daioglou et al. developed the Non-Energy Demand and Emissions (NEDE) model for use in the Integrated Model to Assess the Global Environment (IMAGE),[22] but the NEDE model does not include emerging catalytic production technologies like oxidative coupling of methane (OCM), oxidative dehydrogenation (ODH), and catalytic cracking (CC). The IMAGE team also conducted a multisector analysis exploring decarbonization pathways for heavy industries, including chemical production. This effort projected two paths to net-zero emissions: electrified cracking or CCUS.[23] The pathways represented in their preliminary analysis (reclaimed CO_2 to methanol to olefins, electrified steam crackers, and recycling) lacked additional mitigation strategies, such as the competition between CCS or clean hydrogen with electrified steam cracking. Stegmann et al. recently expanded on the NEDE model to include an exogenous representation of plastics: the plastics integrated assessment (PLAIA) model, which notably demonstrated potential implications of a circular economy and a circular bioeconomy.[24,25] A key limitation of their analysis was a representation of final energy use that aggregated process energy together with feedstocks.

Here, we utilize our expertise to advance the Global Change Analysis Model's (GCAM) portrayal of chemicals to endogenously assess a full suite of decarbonization options for the organic chemical sector.[26,27] Figure 1 serves as a visual orientation to describe the flows of carbon through the system in (a) 2015 and (b) this study's 2050 net-zero CO_2 policy scenario. The system includes upstream production of inputs for feedstock (methanol and refining of fossil and biogenic carbon), process heat (electricity, hydrogen, and fossil or biofuels), and electricity for plastics recycling as part of waste treatment.

The objective is to identify specific actions that the sector can undertake to reduce CO_2 emissions within a broader global context seeking net-zero emissions. Though our presented results focus on CO_2, GCAM also tracks the non-CO_2 GHG emissions associated with the extraction, processing, transmission, and distribution of fossil resources such as gas and oil including methane leakage, venting, and flaring. We consider the most extensive set of organic chemical production technologies examined to date within an IAM, to the best of our knowledge, to see what role each might play in mitigating the sector's CO_2 emissions. We coupled CCS with process heat generation and included alternative process heat technologies (e.g., hydrogen or electricity).[28,29] We also disaggregated the representation of energy inputs into process heat and feedstock, providing valuable detail about trade-offs and opportunities for mitigation.

2. METHODS

2.1. Overview. We updated the structure of GCAM v5.4 to include a detailed representation of organic chemical manufacturing, process heat generation, and methanol production.[30] GCAM is an open-source model developed and maintained at Pacific Northwest National Laboratory's (PNNL) Joint Global Change Research Institute (JGCRI). GCAM is a global model that represents the behavior of, and interactions between, five systems: the energy system, water, agriculture and land use, the economy, and the climate. GCAM is a recursive dynamic model solving for market equilibrium prices and quantities of various resources and markets in 5-year time-steps from 2015 (calibration year) to 2100. Until recently, the industrial sector, apart from cement and fertilizer, was represented as an aggregated consumption of generic energy services and feedstocks.[31]

We first parametrized the incumbent organic chemical manufacturing process: steam cracking. Next, we included alternative organic chemical manufacturing technologies such as ethanol dehydration, OCM, CC, ODH, and methanol to chemicals. Despite the minor variations we know occur across regions due to the commodity nature of the industry, we included globally uniform estimates of cost and performance as model parameters for these technologies.[32] We also added ways to mitigate steam cracking's emissions by considering technologies that can reduce the process heat CO_2 footprint (combustion with CCS as well as switching sources of heat, e.g., to low- or zero-emission electricity or hydrogen) or by using alternative feedstocks sourced from biogenic carbon or plastic scrap. Most of the heat required by the organic chemical sector is classified as hard-to-electrify high-temperature (750–875 °C) heat.[33,34]

Biomass liquids feedstock is exclusively used in ethanol dehydration or as a bionaphtha in liquid cracking technologies. Implicit here is the need for agricultural land, fertilizer, and processing to generate biomass feedstock. The upstream biomass production will have its own emissions of CO_2 as well as other potent GHGs such as N_2O and CH_4, which are accounted for by the integrated framework of GCAM. Finally, we also represent the end-of-life waste treatment of the delivered products that are derived from organic chemicals such as landfilling, incinerating, and recycling.

With this structure, we can track the flow of energy and carbon through the system, as shown in Figure 1, and understand the transitions in (1) process heat generation, (2) organic chemical production technological choice, and (3) feedstock utilization when a CO_2 emissions constraint is applied to the energy and land use systems. The fully coupled nature of the model allows us to evaluate the relative importance of these three (aggregate) process mitigation pathways as well as the effects of waste treatment.

2.2. Production Technologies. We extended the MFA established by Levi et al. for 2013 with additional data from the Oil and Gas Journal (OGJ) to calibrate our model.[9] We aggregated historic steam cracking capacity estimates to regional levels that match those of GCAM's 32 economic regions. For any country with data omitted, the previous year's capacity was used in place of a null value whenever possible. Like Levi et al., we assumed a capacity factor of 85%.[9] This production estimate was further calibrated based on regional

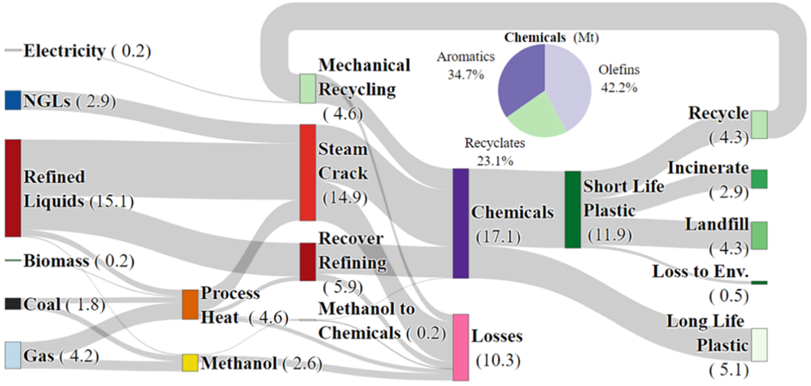

Figure 2. Flow of energy (in exajoules, EJ) as feedstock and process heat through the global organic chemical sector from production to waste treatment in 2015. The numbers in parentheses reflect the flow of energy in EJ. Low-value byproducts from steam cracking are included as losses. Note: the model calculates organic chemical production in mass units (Mt), but for consistency, these have been reported here in energy units (EJ). The assumed lower heating value of chemicals (ethylene, propylene, C4 stream, and aromatics) is 45 GJ/t, that of methanol is 21 GJ/t, and that of plastic is 31.52 GJ/t. In mass units: 72 Mt methanol, 379 Mt organic chemicals, 377.5 Mt short-lived plastics, and 161.8 Mt long-lived plastics. It is estimated that ~5% of short-life plastic (or ~10% of the short-life plastics that are landfilled) is lost to the environment. The pie chart visualizes the mix of final chemicals products. In the pie chart, *recyclates* are intermediate products produced from recycling. A similar Sankey diagram for a net-zero scenario in 2050 is included in the Supporting Information.

energy consumption recorded in the IEA world energy balances' (IEA WEB) chemicals sector data for a given year.[2]

The use of gas liquids for organic chemical feedstocks has grown as a result of unconventional production from shale formations in the U.S.[35−37] In GCAM, gas liquids are considered refined liquids, so we used the IEA WEB to estimate the split between gas liquids (ethane, propane, and butane) and traditional refined liquids (i.e., naphtha) used as feedstock. Disaggregating steam cracking by feedstock was necessary because of regionally dependent availability and deployment, the different specific energy consumptions and product mixes, and the future competition with emerging production technologies. The primary product of steam cracking is ethylene.[9,38] It is best practice that methane coproduced during cracking is used to generate process heat, so we assume this is fully adopted globally by 2050.[39] The other production processes we calibrated in addition to steam cracking involve recovery from refining (e.g., catalytic cracking and catalytic reforming) and methanol to chemicals.[5] We included recovery refining as a portion of steam cracking production based on Levi et al.[9] The primary products from recovery refining are aromatics.[40] We assume historic production of methanol to chemicals in China occurs entirely using coal-based methanol.[9]

2.3. Process Heat. In addition to feedstock requirements, the production of organic chemicals requires energy in the form of high-temperature heat. Careful modeling of the energy used as process heat in the organic chemical sector allows for a more accurate characterization of the likely changes in the sector due to a CO_2 policy, such as, fossil CCS technologies competing with low- to zero-carbon electricity and hydrogen. The parameters we apply in GCAM were derived from a variety of sources.[41−47] We combined a best practice rule from the Department of Energy's (DOE) Better Buildings Initiative with data from the National Renewable Energy Lab's Electricity Annual Technology Baseline (NREL E-ATB) to estimate the cost of industrial boilers.[48,49] We included a 20% decrease in efficiency for CCS technologies relative to their non-CCS counterpart, similar to the assumption made in the Energy Information Administration's (EIA) National Energy Modeling System (NEMS).[50]

2.4. End of Life. We adapted the MFA conducted by Geyer et al. to consider what happens at the end of life for organic chemical products.[7] We assume that all organic chemicals end up as plastics, that the majority (70%) of plastics have short life spans, and that historically, most plastics have been landfilled (58% in 2015). We assume that the carbon contained in landfilled plastics is permanently stored.[51] Our parametrization of this storage begins with a carbon sequestration coefficient initialized to the conversion efficiency (% of feedstock that ends up as organic chemicals) for each technology represented. We adjusted this parameter for the flow of low-value byproducts back to refinery and for the loss of carbon from the incineration of short-lived plastics. Note that there is also carbon lost during recycling, but this is represented as a technology with a conversion efficiency, so it did not need to be considered in the sequestration coefficient of other technologies to avoid double counting.

2.5. Historic Calibration. A Sankey diagram (Figure 2) depicts how energy (in exajoules, EJ) flows through the organic chemical sector (2015 data). The data represented here are the baseline from which we project the future of organic chemical production under a business-as-usual scenario and several CO_2 policy scenarios. The pie chart visualizes the mix of final chemical products. The share of olefins and aromatics is estimated using conversion matrices provided by Neelis et al. for steam cracking.[39] The mix of organic chemicals varies with the operational conditions (temperature and pressure). For this reason and to limit model complexity, GCAM tracks organic chemicals at an aggregated level. Organic chemicals conversion to final products was qualitatively described here as long or short life with the short-life component also used for an estimate of the end-of-life treatment.[7]

2.6. Scenario Design. In the base scenario, we assume that global plastics waste treatment converges toward the method used in the most advanced countries, such as Norway. These countries have about a 60:40 split between plastic incineration and recycling, with little to none of the final products being disposed of in landfills.[52] The future demand for organic chemicals (olefins, aromatics, and methanol) was estimated with an income elasticity and further constrained with a price

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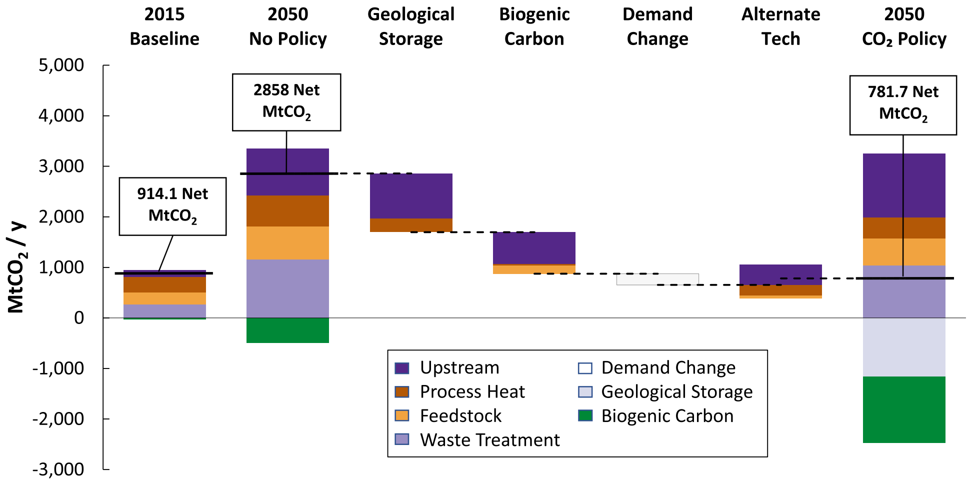

Figure 3. Net CO_2 emissions reductions in million metric tons (Mt CO_2) per year for the global organic chemical sector under an economy-wide net-zero CO_2 constraint by 2050 with our base waste treatment assumptions. The top-down orientation and color scheme of this figure corresponds to the carbon flow depicted in Figure 1. In our base scenario, the share of plastic waste incinerated is projected to increase from 22 to 60% of short-lived products. We assume 100% of carbon in the product is lost during incineration. Sources of CO_2 emissions include upstream production, process heat generation, feedstock conversion, and waste treatment. Sources of CO_2 emissions are offset by the permanent sequestration of CO_2 in geological storage and the use of biogenic carbon. The differences between the scenarios' emissions are categorized by mitigation strategy and traced to stages of the life cycle. Dashed lines show the steps down from left to right. A solid black line is used to mark the net emissions. Additional CO_2 emissions results for the main and supplementary scenarios are included in the Supporting Information.

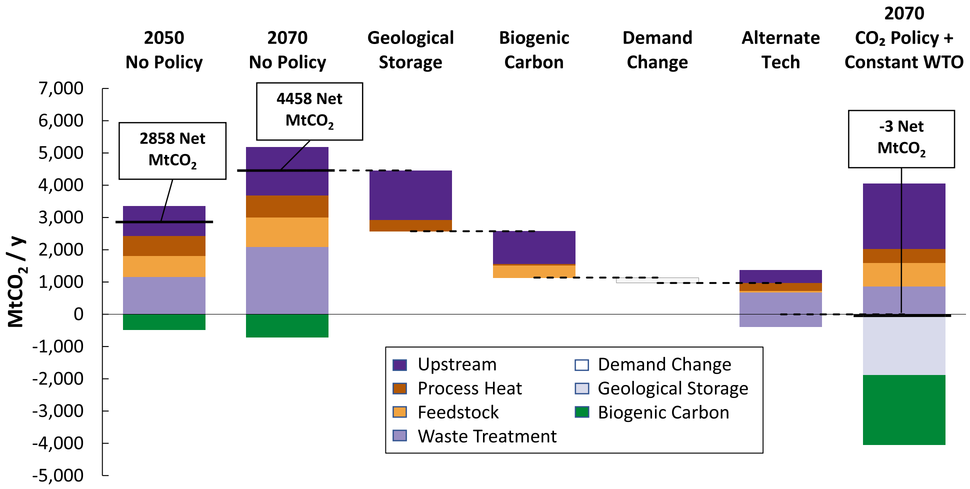

Figure 4. Net CO_2 emissions reductions in million metric tons (Mt CO_2) per year for the global organic chemical sector under an economy-wide net-zero CO_2 constraint by 2070 with waste treatment held constant at 2015 levels. The top-down orientation and color scheme of this figure corresponds to the carbon flow depicted in Figure 1. In our constant WTO scenario, the 2015 reference point is 22% incineration, 58% landfill, and 20% recycle. Note: the share of landfill includes an estimated 5% of plastic that is released to (and stored in) the environment due to dumping or improperly landfilled materials. Sources of CO_2 emissions include upstream production, process heat generation, feedstock conversion, and waste treatment. Sources of CO_2 emissions are offset by the permanent sequestration of CO_2 in geological storage and the use of biogenic carbon. The differences between the scenarios' emissions are categorized by mitigation strategy and traced to stages of the life cycle. Dashed lines show the steps down from left to right. A solid black line is used to mark the net emissions. Additional CO_2 emissions results for the main and supplementary scenarios are included in the Supporting Information.

elasticity. We generated an income elasticity curve for organic chemicals based on data from Daioglou et al.,[22] but further calibrated those income elasticities to match updated projections of the sector's growth.[5−8]

Our reference (or "baseline no-policy") scenario applies a "Middle of the Road" shared socioeconomic pathway (SSP2), which assumes future demographic, economic, technological, and behavioral developments that are in line with historical patterns.[53,54] Building on this SSP2 baseline, the net-zero CO_2 scenarios also apply an economy-wide constraint via an endogenously solved CO_2 price to meet the constraint. The global economy-wide CO_2 constraint begins in 2025 and decreases linearly to zero emissions by 2050 and further to −10,000 Mt CO_2 per year by 2100. This constraint results in global mean temperature change from preindustrial to well below + 2 °C by 2100 while using the default climate model in GCAM, Hector.[55] We also ran a constant waste treatment option (WTO) scenario, where the global shares of landfilled, incinerated, and recycled products do not change from 2015 values. The WTO scenario is the only scenario that reaches a net-negative CO_2 emissions future for the organic chemical sector. We evaluated the sensitivity of the modeled organic chemical CO_2 emissions to several key parameters. Our sensitivity analysis determined the effect of a 30% increase and decrease to the original values of the following GCAM parameters: the extent of geological CO_2 storage, the consumer demand for organic chemicals, the price of oil, the use of biogenic carbon as a feedstock, the share of long-lived products, the share of incineration, and the share of recycling.

The Supporting Information includes a flowchart depicting sources of emissions during the production of organic chemicals (Figures S2 and S6), a discussion of chemical production technology and process heat parameters (Tables S1−S3 and Figure S3), a discussion of the model calibration process and the results of the calibration for steam cracking and methanol production (Figures S4, S5, and S7), and additional scenario details (Table S4 and Figures S9, S10, and S12).

3. RESULTS

3.1. Deployment and Impact of Emissions Reduction Strategies.

We use waterfall charts to highlight the life cycle stages where specific mitigation strategies are deployed. Sources of CO_2 emissions include upstream production, process heat generation, feedstock conversion, and waste treatment. The upstream production of inputs into the organic chemical sector includes electricity, hydrogen, refining, and methanol. Emissions from waste treatment include recycling and incineration. Sources of CO_2 emissions are offset by the deployment of CCS resulting in the permanent sequestration of CO_2 in geological storage and the use of biogenic carbon.[56,57] CCS (and therefore geological storage) can be implemented during the upstream production and process heat generation. Biogenic carbon can influence emissions at any stage. Other strategies to mitigate emissions include demand reduction, shifts in waste treatment, and the increased use of more energy/conversion efficient technologies during upstream production, process heat generation, and feedstock conversion. The model tracks non-CO_2 GHG emissions such as methane leakage. Methane emissions decline under a CO_2 policy due to the reduced flow of gas into the system and as the price of GHG emissions induces emission reductions along the marginal abatement cost curves.[58] Figures 3 and 4 only plot CO_2 emissions, but more information about non-CO_2 emissions trends is included in Figure S11.

Figure 3 presents the net CO_2 emissions reductions of the global organic chemical sector under an economy-wide net-zero CO_2 constraint in 2050 with our base waste treatment assumptions. The no-policy and CO_2 policy scenarios share the same base waste treatment assumptions to prevent changes in this stage from impacting the total emissions reductions between the two scenarios. In our base scenario, the share of plastic waste incinerated and, therefore, 100% of carbon in the product lost is projected to increase from 22% to 60% of short-lived products.

Figure 3 shows that, absent any further climate policy, modeled sector emissions increase more than 3 times 2015 levels by midcentury. The emissions increase by midcentury is roughly equivalent to the relative increase in organic chemicals produced (and associated demand). The largest difference between 2015 and 2050 is due to increased upstream production of methanol as a feedstock and assumptions about the future trajectory of waste treatment. We see from the next full bar that a global CO_2 policy reduces 2050 emissions by ∼73%, but only ∼15% compared to 2015. So, under an economy-wide net-zero CO_2 policy, the model offsets residual organic chemical sector emissions rather than implementing additional mitigation measures to bring the system to zero net CO_2 emissions by midcentury.

The 2050 net CO_2 emission reductions attributable to the CO_2 policy arise from geological storage of CO_2 (∼52%), increased use of biogenic carbon (∼37%), and demand reduction (∼10%). The introduction of alternative technologies does not contribute to reductions between the scenarios because relatively modest mitigation for process heat and conversion is more than offset by an upstream increase in hydrogen production and the less efficient production of biomass liquids. We recognize that a future reliant on such a large deployment of geological storage (CCS) is uncertain, and this finding is further tested in our sensitivity analysis. Organic chemical production falls under a net-zero CO_2 policy compared to the reference scenario. The combination of geological storage and biogenic carbon reductions in upstream production emissions results in net-negative emissions inputs into the organic chemical sector. Upstream emissions are reduced through the deployment of CCS, and total emissions can become negative with the combination of biogenic carbon and CCS. Upstream mitigation accounts for ∼54% of the net emission reductions observed between the no-policy and net-zero CO_2 policy scenarios at midcentury.

We find that the combination of strategies deployed to reduce emissions from organic chemical process heat accounts for ∼24% of the net emission reductions due to the CO_2 policy. Process heat coupled to CCS accounts for 55% of these reductions. Other strategies include the use of biogenic carbon as a fuel for process heat (∼5%) and an increased deployment of alternative process heat technologies (∼40%), such as low- or zero-emission hydrogen and electricity, compared with the no-policy case. Next, we find that reductions in feedstock emissions account for ∼11% of the net emission reductions due to the CO_2 policy. An increased use of biogenic carbon as a feedstock for organic chemical production is responsible for 71% of the observed reductions in the level of feedstock emissions. Alternative technologies account for the remaining reductions. This reveals that the path to decarbonize process heat is more cost-effective than the path for emissions from carbon feedstock, as the latter shows a smaller reduction by 2050.

Figure 4 details the potential to further reduce sector emissions from a net of 781.7 Mt CO_2 in 2050 to a net of 0 Mt CO_2 in 2070 when waste treatment shares are held constant at 2015 levels. This was the only scenario that reduced the net CO_2 emissions of the organic chemical sector to zero or below. In our constant WTO scenario, the 2015 reference point is 22% incineration, 58% landfill, and 20% recycle. Note: the share of landfill includes an estimated 5% of plastic that is released to (and stored in) the environment due to dumping or improperly landfilled materials.[59] Assuming no biodegradation in landfills, biogenic carbon as a feedstock for organic chemicals that end up as short-life plastics results in negative emissions when landfilled. While such a future produces a desirable outcome in terms of emissions, waste treatment futures raise additional environmental and sustainability concerns such as microplastics accumulation in the environment from direct dumping or improperly landfilled material.[60−63]

The results shown in Figure 4 demonstrate increased geological storage, increased use of biogenic carbon, lower

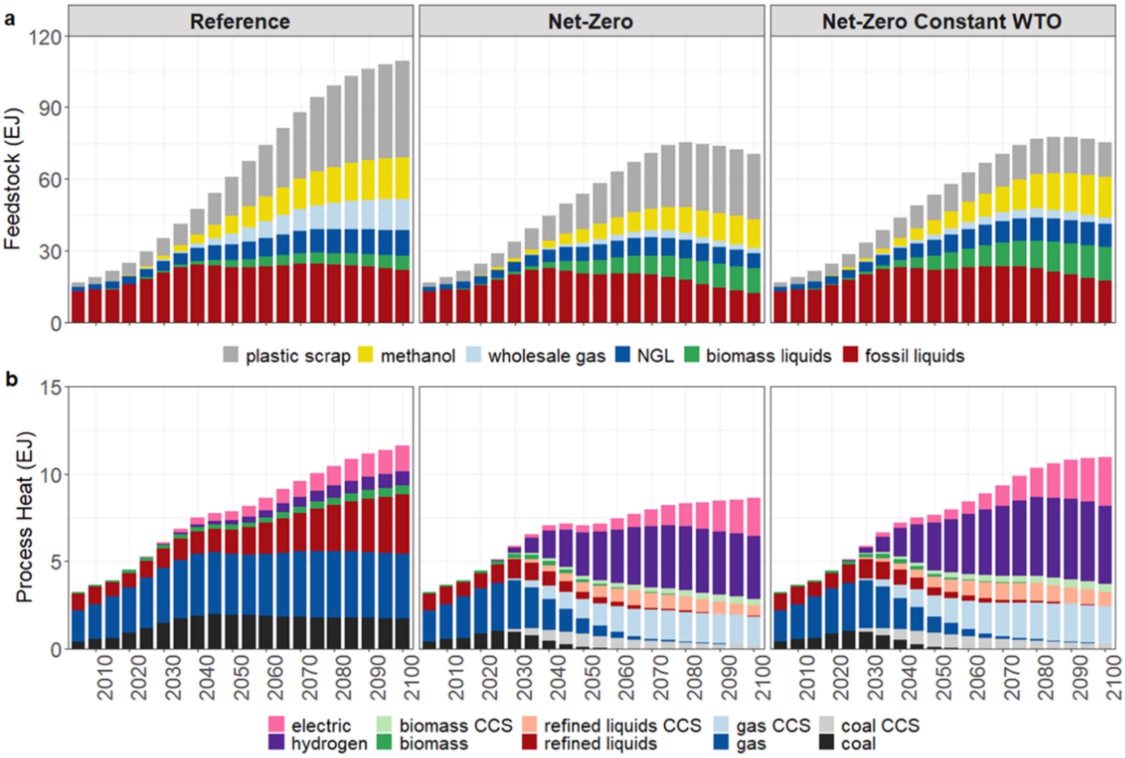

Figure 5. Global transitions in the organic chemical sector in exajoules (EJ), (a) Feedstock and (b) process heat, to 2100 under different scenarios. "NGL" refers to gas liquids. CCS refers to carbon capture and storage. This figure compares the same net-zero CO_2 policy scenarios, introduced in Figure 3, impacting energy use within the organic chemical sector. Each panel has three graphs that represent the three main scenarios of this analysis: a reference ("no-policy"), a net-zero CO_2 policy, and a net-zero CO_2 policy with constant waste treatment options (WTO). Note: the panels have the same units (EJ) but different scales. Feedstock and process heat charts for four additional scenarios are included in the Supporting Information.

demand reduction, and reductions in waste treatment emissions. The increased deployment of geological storage and use of biogenic carbon in upstream processes are partially offset by an increase in the less efficient production of biomass liquids and methanol. Process heat and feedstock emissions continue to be reduced with the same strategies already noted (i.e., clean hydrogen, renewable electricity, and biomass, as well as more CCS-based technologies). We see a significant reduction in the emissions from waste treatment as the share of incineration remains lower than our base assumptions. Finally, we also see a slightly smaller contribution in reductions from changes in demand compared with Figure 3.

3.2. Feedstock, Process Heat, and Technological Transitions. Figure 5a visualizes transitions in feedstocks for the organic chemical sector. In all scenarios, feedstocks from fossil sources continue to hold a major share by midcentury and all the way to 2100 for the reference and net-zero WTO scenarios. Alternative feedstocks such as plastic scrap, methanol, and biomass liquids gain the major share in 2085 of the base net-zero scenario. This result further clarifies the conclusion, drawn from Figure 3, that emissions from feedstock are hard to mitigate. In the net-zero scenarios, the amount of feedstock is lower than the reference because of reduced production in response to the CO_2 policy. We also find that the net-zero scenarios use more biomass liquid feedstock than the reference case. The amount of biomass liquids used as feedstock grows in the net-zero constant WTO scenario in response to the net-negative emissions produced by the permanent storage of biogenic carbon in organic chemical products via landfilling. We discuss in further detail below the sensitivity of our results to the amount of biogenic carbon used as feedstock and the price of oil. The majority of methanol used as feedstock is produced from fossil carbon. However, these results depend on the future demand of methanol; for example, if there is a large demand for low-emission methanol as a shipping fuel, the technologies that use biomass or reclaimed CO_2 may advance quickly to replace fossil carbon.[64] In the reference scenario, there is a large amount of gas feedstock in response to the deployment of the OCM technology. But gas feedstock is not as prominent in the net-zero scenarios primarily because of the poor conversion efficiency of OCM.

Figure 5b visualizes transitions in process heat generation for the organic chemical sector. We find that the growth in process heat in the reference scenario comes from refined liquids and gas primarily based on historic regional fuel preference and availability. The amount of process heat generated in the net-zero scenarios is lower than that in the reference. This reduction is due to lower demand for organic chemicals in response to the CO_2 constraint, which is partially offset by the efficiency loss from CCS. The net-zero constant WTO requires more process heat than the base net-zero case as the lower energy-demanding mechanical recycling technology has a smaller share of production. In both net-zero scenarios, heat generation from alternative technologies (hydrogen and electricity) holds the majority by 2045, while deployment of heat generation with CCS follows close behind. The amount of electric or hydrogen process heat deployed partially depends on the rate of decarbonization in the respective sector. Regardless of the deployment of alternative technologies, these

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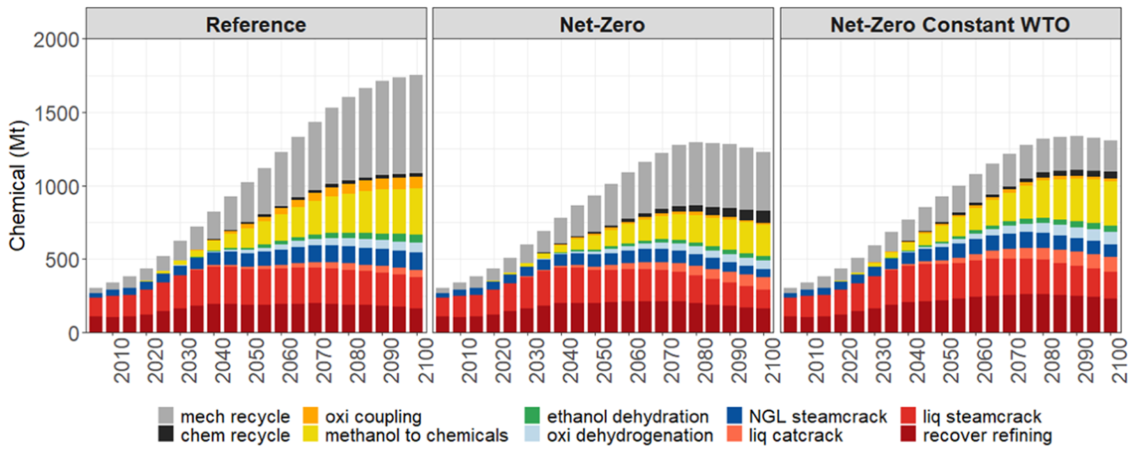

Figure 6. Global production technology transitions in the organic chemical sector in million metric tons (Mt) to 2100 under different scenarios: reference, net-zero, and net-zero with waste treatment held constant at 2015 shares. mech, mechanical; chem, chemical; oxi, oxidative; NGL, gas liquids; liq, liquid; catcrack, catalytic cracking. This figure compares the same net-zero CO_2 policy scenarios, introduced in Figure 3, with impact on production technologies within the organic chemical sector. Production technology charts for four additional scenarios are included in the Supporting Information.

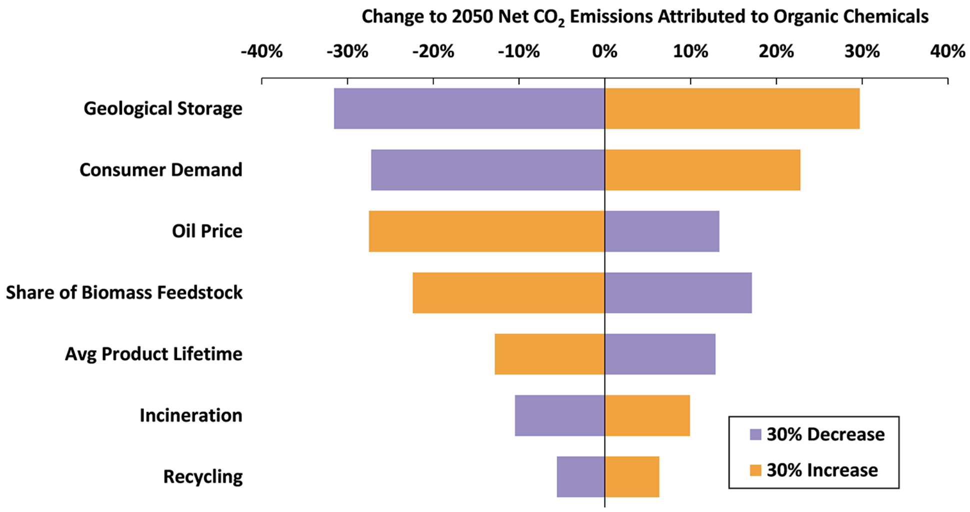

Figure 7. Sensitivity analysis of the net organic chemical sector CO_2 emissions to assess the impact of systematic perturbation on baseline emissions. Each parameter was increased (orange bar) or decreased (purple bar) by 30% relative to the baseline net-zero scenario in 2050. The direction of these bars represents the impact of the change in parameter value on net CO_2 emissions, relative to the base net-zero scenario's organic chemical sector's net emissions. Bars to the left reflect a decrease in emissions, and bars to the right reflect an increase in emissions. Wider bars are indicative of greater sensitivity in modeling output.

results are somewhat at odds with the prevailing view in the industry that process heat will be fully electric within a few decades.[22,23]

Figure 6 visualizes the transitions in production technology for the organic chemical sector. As highlighted in Figure 3, these are less effective than changes to energy used to generate process heat and as feedstocks in response to a CO_2 policy. The production of organic chemicals in the net-zero scenarios is lower than the reference scenario. Without sufficient mitigation options, the sector is forced to reduce production as demand decreases in response to increased product costs. In fact, we observe a decrease in the volume of organic chemicals produced compared to the reference case for every net-zero scenario except for the net-zero circular bioeconomy. Chemical recycling (pyrolysis of plastic scrap), which was parametrized based on the LCA of Yadav et al. never gains a significant market share in this analysis.[65] However, emerging policies such as fixed recycling ratios or the production of commodities other than chemicals (e.g., naphtha) could result in a larger deployment of chemical recycling.[66] And although OCM deploys under the reference scenario, its use is dampened in the net-zero scenarios. This is due to the poor conversion efficiency of OCM—modeled here as 30%, which is considered a commercially viable target.[67] Furthermore, in all scenarios, we observe a slow introduction of alternative production technologies, most notably, methanol to chemicals, ODH, and CC. The preference for these catalytic processes is based on moderate gains in energy consumption and conversion efficiency. In the net-zero scenarios, these new technologies slowly take market share away from incumbent steam cracking. But thermodynamics limits the savings potential of catalysts, which could also bring up indirect trade-offs under a systems expansion when considering the mining of critical minerals that these technologies generally require.

3.3. Sensitivity Analysis. Figure 7 presents the results of a sensitivity analysis that assesses the impact of systematic perturbation on baseline CO_2 emissions. We selected key parameters, and each was increased (orange bar) or decreased (purple bar) by 30% relative to the base net-zero scenario in 2050. The direction of these bars represents the effect of the change in parameter value on net CO_2 emissions, relative to the base net-zero scenario's organic chemical sector's net emissions. Wider bars are indicative of greater sensitivity in the modeling output.

Organic chemical sector emissions are most sensitive to the extent of geological CO_2 storage and consumer demand. When base geological storage is 30% higher, net organic chemical sector CO_2 emissions are higher. The increase is caused by less biogenic carbon used in the organic chemical system. Furthermore, the increase is offset by an increase in geological storage in other parts of the economy, most notably during the production of hydrogen from biomass and coal. Conversely, when base geological storage is 30% lower, net organic chemical sector CO_2 emissions are lower. This decrease is the result of the increased use of biogenic carbon in refining and as feedstock for organic chemicals. We noted in the discussion of Figure 3 that the production of organic chemicals decreases between a reference and both economy-wide net-zero scenarios. To assess the impact of demand for organic chemicals on net CO_2 emissions for the sector, we further tested the effects of forcing either higher or lower organic chemicals production volume. The impact is as expected: when the organic chemical production volume is high, net CO_2 emissions are higher.

When oil prices are higher, the sector's net CO_2 emissions are lower. Production of biomass liquids and, therefore, the use of biogenic carbon as a feedstock, increases in response to higher oil prices. The low oil price sensitivity is the only parameter for which the sensitivity results are not symmetrical. The model exhibits a greater reduction in CO_2 emissions per 30% increase in oil price compared to a smaller increase in CO_2 emissions per 30% decrease in oil price. This result suggests that in a world where oil prices are low, it will be economically efficient for the organic chemical sector to find different ways to mitigate emissions than by using biogenic carbon feedstock.

We also tested the impact of product lifetime by increasing and decreasing the share of long-lived products as estimated by Geyer et al.[7] When the share of long-lived products increases, the net CO_2 emissions decrease. When the share of long-lived products decreases, the net CO_2 emissions increase. This exercise was primarily conducted to evaluate the uncertainty of product lifetime estimates rather than to suggest it is feasible for decision makers to influence the lifetime of organic chemical sector products. But standards and policies on biodegradable plastics could have similar effects. Finally, we tested the sensitivity to additional changes in waste treatment options. When either the share of incineration or recycling increases, net emissions increase. Both results from waste treatment sensitivities are dependent upon the amount of carbon permanently stored in plastics in landfills.

The Supporting Information includes results for additional scenarios (Figures S13−S17) and an energy Sankey for the net-zero scenario in 2050 (Figure S18).

4. DISCUSSION

Our representation of global organic chemical production endogenously tracks the flow of energy and carbon in an IAM. This allowed us to assess the full suite of mitigation strategies for the sector. The results of this study are limited by the data and assumptions made to calibrate the model, which we tried to assess via a sensitivity analysis and additional scenarios. For example, with limited publicly available data about the production and consumption of chemicals, we made assumptions about demand. Demand was one of the parameters that net CO_2 emissions of the organic chemical sector was most sensitive to. Other limitations include our assumptions about waste treatment, but changes to these assumptions had the least impact on our sensitivity analysis. Finally, we used uniform parameters of non-energy cost and efficiency across regions and time. We recognize that some of the technologies we included could experience improvements in both parameters as they are further developed. We included results for an additional scenario that estimates these improvements in the Supporting Information.

This analysis is also limited by the use of a uniform global carbon price, which is a common surrogate for real-world policy in IAM simulations but which often fails to capture the regional variation of policy implementation actually observed. Future work should also incorporate a consideration of biodegradable plastics, a further representation of intermediate organic chemical to final plastic polymer product, and an additional investigation of the future trends and emerging technologies for the waste treatment of plastics that expands upon what has already been considered in our analysis. However, our results make clear that absent any additional climate policy, net sectoral emissions increase more than 3 times 2015 levels by midcentury.

We found that a net-zero CO_2 by 2050 policy only reduces emissions by 15% compared to 2015. Furthermore, results showed that upstream emissions associated with the inputs of refining, methanol, hydrogen, and electricity are net negative; process heat emissions are reduced by ∼76%, and feedstock emissions (including waste treatment) are reduced by 18% (both compared to 2050 reference levels). The detail with which we model the organic chemical sector is critically important because it allows us to assess cost trade-offs in ways that were not possible before. Once we take these trade-offs into account, we reveal several key new results about decarbonizing the sector.

Geological carbon storage deployed upstream and during the generation of process heat accounts for about half of the observed mitigations in the organic chemical sector. Additionally, 55% of the mitigated emissions from process heat by midcentury are the result of geological carbon storage. Alternatives to CCS-based process heat, like low- to zero-carbon electricity or clean hydrogen, account for the remaining reductions. We recognize that a future reliant on such a large deployment of CCS faces uncertainty, but this result arises from the costly trade-offs that would be required by other pathways. Our sensitivity analysis revealed that the global organic chemical sector relies on more biogenic carbon to reduce emissions when the availability of geological storage is reduced.

Biogenic carbon accounts for ∼30% of the total emissions mitigations in the sector. The combination of geological carbon storage and biogenic carbon significantly decarbonizes

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upstream production, resulting in net-negative inputs into the organic chemical sector. Consistent with Stegmann et al., our results indicate that the combination of an increase in biogenic carbon as a feedstock for organic chemicals and a high share of landfilled waste treatment of plastics enables the sector to deliver net-negative emissions,[25] although such a future raises other environmental and sustainability concerns. We can also conclude that alternative feedstocks must have a larger share of the pie if greater reductions are to be seen in the sector. Although alternative feedstocks other than biogenic carbon exist, such as chemicals from advanced recycling or reclaimed CO_2, these options are not found to be economically viable in our results.

■ ASSOCIATED CONTENT

Data Availability Statement

GCAM is an open-source integrated assessment model available at https://github.com/JGCRI/gcam-core (version 5.4). Additional scenario inputs are summarized in the Supporting Information. The full set of input files and source code associated with this study as well model output data and source data for figures are available at 10.5281/zenodo.10018520.[68]

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.est.3c05202.

> Flowcharts depicting sources of emissions during the production of organic chemicals; detailed discussion of chemical production technology parameters, process heat parameters, model calibration process, and the results of the calibration for steam cracking and methanol production; additional scenario details; results for additional scenarios; and an energy Sankey for the net-zero scenario in 2050 (PDF)

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Notes

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■ ABBREVIATIONS

GJ=gigajoules
EJ=exajoules
t=metric tons
Mt=million metric tons

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