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Decarbonization pathways for liquid fuels: a multi-sector energy system perspective

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Low-carbon liquid fuels play a key role in energy system decarbonization scenarios. This study uses a multi-sector capacity expansion model of the contiguous United States to examine liquid fuels production in deeply decarbonized energy systems, using representations of multiple liquid fuel pathways with harmonized carbon and energy balances to enable consistent system-level comparison across technologies. Our analysis evaluates how the shares of biofuels, synthetic fuels, and fossil liquid fuels change under varying assumptions about resource constraints (biomass and CO_2 sequestration availability), fuel demand distributions, and supply flexibility to produce different fuel products. Across all scenarios examined, biofuels provide a substantial share of liquid fuel supply, while synthetic fuels deploy only when biomass or CO_2 sequestration is assumed to be more limited. Fossil liquid fuels remain in all scenarios examined, primarily driven by the extent to which their emissions can be offset with removals. Limiting biomass increases biogenic CO_2 capture within biofuel pathways, while limiting sequestration availability increases the share of captured atmospheric (including biogenic) carbon directed toward utilization for synthetic fuel production. While varying assumptions about liquid fuel demand distributions and fuel product supply flexibility alter competition among individual fuel production technologies, broader energy system outcomes are robust to these assumptions. Biomass and CO_2 sequestration availability are key drivers of energy system outcomes in deeply decarbonized energy systems.

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1. Introduction

Liquid and gaseous fuels dominate final energy demand in current energy systems. For example, liquid and gaseous fuels represented 70% of final energy use in the U.S. in 2023.[1] While electrification of building, industrial, and transport end uses is projected to increase over time, particularly under deep decarbonization, energy system modeling consistently shows a continued role for gaseous fuels such as methane and liquid hydrocarbon fuels in net-zero energy systems.[2–7] This persistence is largely due to the prevailing technological challenges of electrifying certain end uses such as heavy-duty transport, aviation, marine shipping, and high-temperature industrial processes.[8–10] Moreover, because fossil-derived liquid fuels are generally more carbon-intensive and costly on a per-energy basis than fossil gaseous fuels (*e.g.*, methane),[3] there are stronger economic incentives under carbon pricing to develop and adopt alternative production routes for liquid fuels than to deploy analogous options for gaseous fuels.

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Multiple technology options can reduce emissions associated with the use of conventional liquid fuels. These include: (1) deployment of carbon dioxide (CO_2) removal (CDR) technologies, such as direct air carbon capture and sequestration (DACCS) or bioenergy with carbon capture followed by sequestration (BECCS), to offset emissions from continued use of fossil liquids,[11–13] (2) the conversion of biomass to liquid fuels (biofuels), and (3) the production of synthetic fuels using hydrogen (H_2) and captured atmospheric CO_2, including captured biogenic CO_2.[14] Assessing the relative competitiveness of these liquid fuel pathways is challenging for several reasons. First, liquid fuel production pathways span a range of technological processes (*e.g.*, refining, pyrolysis, and gasification followed by Fischer–Tropsch (FT) or methanol synthesis, among others), feeds (*e.g.*, oil, multiple forms of biomass, hydrogen, and CO_2), and energy inputs (*e.g.*, electricity and natural gas). In FT-based pathways, syngas intermediates (primarily hydrogen and carbon monoxide) are formed and subsequently converted into liquid hydrocarbons. Second, large-scale deployment of alternative fuel pathways would create new cross-sectoral interactions within the energy system – for instance, the increased demand for hydrogen and captured CO_2 associated with synthetic fuel production, related demands for electricity, and corresponding infrastructure requirements.[15]

Several prior studies have undertaken techno-economic analysis (TEA) of biofuel and synthetic fuel production routes, with a focus on comparing process cost outcomes under various technology and input assumptions.[16–21] These studies provide an engineering basis to quantify performance of pathways using different processes or feeds, including carbon and energy flows, feed requirements, and product distributions. These studies also highlight the sensitivity of process cost to feed and energy prices (*e.g.*, electricity, H_2, CO_2, biomass) and co-product revenues (*e.g.*, captured CO_2, light hydrocarbons), with one example being the importance of H_2 prices on synthetic fuel production costs.[22] However, TEA studies are unable to assess how resource constraints, such as limited biomass availability, coupled with cross-sectoral interactions, could impact process economics and in turn technology deployment. For example, under deep decarbonization scenarios, biomass used for liquid fuel production may face competition from other sectors such as power generation, driving up its price and consequently the cost of biofuels. Similarly, the price of H_2 for synthetic fuel production depends on the mix of H_2 production technologies deployed and may be weakly or strongly affected by electricity price dynamics, depending on the extent of electrolyzer deployment.[23–25]

In this context, energy system models that account for competing uses of resource-constrained feedstocks and energy commodities across multiple sectors can complement TEAs in understanding fuel technology pathways under various technology and policy assumptions. Many different analysis frameworks have been used to evaluate the role of liquid fuel production technologies in regional or national decarbonization scenarios, such as system dynamic models (SDM),[26–28] integrated assessment models (IAMs),[29–34] and capacity expansion models (CEMs).[35–40] System dynamics models (SDMs) capture feedback-driven dynamics and industry development at a sectoral or regional scale, while integrated assessment models (IAMs) span multiple regions and sectors, linking energy, land, and climate systems with the economy to explore long-term global mitigation pathways. In contrast, CEMs focus on cost-optimal investment and operation of infrastructure, typically at high temporal and technological resolution, making them well suited for analyzing sectoral interactions (*e.g.*, linkage between power and other sectors) and the detailed pathways required for alternative fuel production.

Recent energy system studies[2,3,26,29,35,39,41] of liquid fuel decarbonization pathways illustrate how the competitiveness of alternative fuel production technologies is affected by assumptions about biomass and CO_2 sequestration availability as well as by the stringency of the emissions constraint. Key insights arising from these studies in the context of deep decarbonization include: (a) the potential for competing uses of biomass across fuels and other sectors (*e.g.*, power) depending on technology, demand, and resource availability assumptions,[26,29,35,39,41] (b) the sensitivity of synthetic fuel deployment to assumptions about CO_2 sequestration availability, with greater deployment of such fuels observed in scenarios with limited sequestration availability,[35,39,41] and (c) the continued role of fossil liquid supply to meet demand, along with deployment of CDR technologies to offset remaining emissions.[2,3,35,41]

Despite these advancements, understanding fuel decarbonization pathways and their energy system drivers is limited by several gaps. First, most studies treat liquid fuels as a lumped commodity, even though demand for liquid fuels involves multiple fuel types – primarily gasoline, diesel, and jet fuel, with distinct demand drivers and competing technologies. For instance, although gasoline currently dominates liquid fuel demand in many regions, a combination of technological trends, including growing electrification of light duty vehicles (LDV), could lower the share of gasoline in total liquid fuel demand in the future. This raises a question about how changes in the liquid fuel demand distribution would affect deployment of fuel production technologies.

A second related gap is the lack of adequate consideration of flexibility in fuel product slates from existing fossil liquids and alternative fuel production routes. For instance, petroleum refining assets in the United States and many other regions currently produce gasoline-heavy product slates.[42,43] Although some operational changes can broaden the range of product slates served by existing refineries,[42] substantial changes could require further investments to retrofit these assets. These considerations raise important questions regarding the extent to which new investment could align supply and demand for particular products,[2,3] particularly under deep decarbonization scenarios in which the fuel demand distribution could be different from today.

Similarly, for alternative fuel pathways using biomass and CO_2 feedstocks, TEA studies assume specific fuel product slates, but the impact of changing product slates on process-level cost and performance has not been fully characterized. Moreover, existing energy system studies often do not consider different rates of carbon conversion or CO_2 capture (CC) during biofuel production.[2,3,44] A related challenge for utilizing biofuel TEA data in energy system models is the lack of harmonization of the different feedstock and product composition assumptions used across studies.

Here we address the limitations identified above to enhance understanding of liquid fuel production pathways in cost-optimized, deeply decarbonized energy systems. Our approach utilizes a multi-sector CEM that includes the electricity, H_2, CO_2, biomass, liquid fuels, and natural gas (NG) supply chains. For liquid fuels, we represent 11 alternative fuel production processes with varying cost and performance assumptions, including different CC rates and fuel product distributions. This implementation involves: (a) harmonizing carbon and energy balances for different fuel technology pathways reported in the literature (details in Section S2.3 of the SI); and (b) developing a simple but general method to estimate the costs and energy requirements associated with varying CC rates when such data are not provided by the literature source (details in Section S2.2 of the SI). This approach enables more consistent cross-technology comparisons and shows how system-level assumptions affect the deployment of different liquid fuel pathways under emissions constrained scenarios. Additionally, we explicitly differentiate fuel product demands and impose constraints on fossil liquid product distributions based on historical refinery data, thereby allowing us to quantify how these constraints affect fossil liquid deployment across a range of possible future energy systems.

We apply the framework to a case study of the contiguous United States under a net-zero CO_2 emissions constraint, varying assumptions about biomass and CO_2 sequestration availability (which could reflect resource constraints as well as other factors), the flexibility of supply technologies to alter product mixes, and fuel demand distributions. Our results highlight a substantial role for biofuels with CCS in deeply decarbonized energy systems, with the extent of CO_2 capture within biofuel pathways primarily driven by biomass resource assumptions. Synthetic fuels deploy in several cases, particularly when CO_2 sequestration availability is limited, leading to greater utilization of biogenic CO_2, which effectively intensifies biofuel production. Additionally, while the flexibility of fossil liquids production and the liquid fuels product distribution do not strongly affect overall energy system results, these assumptions significantly affect the competition among individual biofuel processes.

The remainder of this paper is organized as follows. Section 2 outlines the modeling framework, input assumptions, and scenario design with details included in the SI. Section 3 presents the key results from the core energy system scenarios and discusses the sensitivity to alternative demand assumptions, alternative fuel production flexibility assumptions, and alternative techno-economic assumptions. Section 4 discusses the implications for liquid fuel decarbonization strategies and directions for future research, and Section 5 concludes the paper.

2. Methods

2.1. Energy system modeling approach

This study builds upon and extends an open-source, multi-sector CEM, MACRO,[45] to study liquid fuel decarbonization under emissions constraints, summarized in Fig. 1. The model is formulated as a single year cost-optimization that minimizes the sum of system-wide annualized capital and operating costs, spanning the supply chains of electricity, H_2, CO_2, biomass, liquid fuels, and NG. Supplies and demands of these vectors are balanced at the hourly and regional level unless otherwise indicated.

In this study, we expanded MACRO to include representations of liquid and gaseous fuel supply chains and their integration with the rest of the energy system. This includes enforcing supply-demand balances for individual liquid fuels (gasoline, jet fuel, diesel) and NG, as well as introducing investment and operation decisions and constraints for respective production technologies. The model incorporates multiple fuel (both gas and liquids) production pathways, including: (1) biofuels, (2) synthetic fuels synthesized from captured CO_2 and H_2, and (3) continued use of fossil fuels (gas

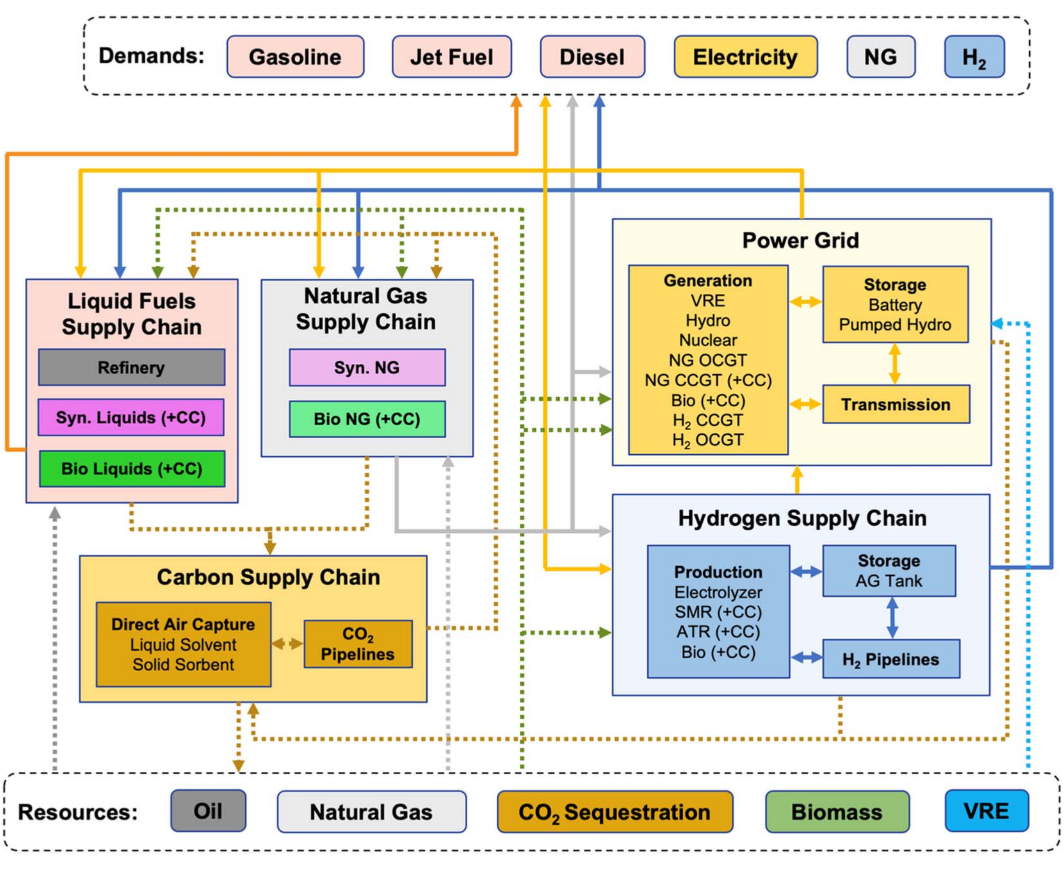

Fig. 1 Architecture of the MACRO model showing the various sectors represented (refer to Section S5 of the SI for model formulation). Key exogenous inputs to the model are highlighted in the dotted boxes labeled "Resources" and "Demands". CC = CO_2 capture, NG = natural gas, VRE = variable renewable energy (solar and wind), OCGT = open cycle gas turbines, CCGT = combined cycle gas turbines, SMR = steam methane reforming, ATR = autothermal reforming, AG = above ground storage, Syn. = synthetic.

and liquids). For biofuel and synthetic fuel pathways, the model resolves the individual fuel outputs and tracks the disposition of unconverted CO_2, which may be either captured or vented depending on the process configuration. To reflect refinery product distribution constraints, the model imposes bounds on the relative outputs of fossil-derived jet fuel, gasoline, and diesel (eqn (S18) and (S19) in Section S5.1).[43] In addition, the model tracks fuel use in other commodity supply chains, such as NG consumption for electricity generation, H_2 production, or direct air capture (DAC).

Resource availability for variable renewable energy (VRE), CO_2 sequestration, and biomass are defined *via* supply curves for each region as described further below. In addition, electricity, H_2, and captured CO_2 can be transported between regions *via* transmission networks and pipelines, subject to capacity limits. Transportation within a region is not represented explicitly, with production and demand assumed to be co-located. This reflects spatial aggregation rather than the absence of local infrastructure costs. Certain intra-regional transmission costs (*e.g.*, VRE grid interconnection) are implicitly included in technology cost assumptions. The model represents existing electricity transmission infrastructure and allows for endogenous investment in additional electricity lines and new pipelines for H_2 and CO_2 when cost-effective. NG transmission is not modeled explicitly; instead, we assume exogenous NG prices at the regional level, which implicitly accounts for differences in transmission costs. Liquid fuel transmission costs are implicitly assumed to be small by enforcing the supply-demand balance at the national level rather than the regional level (eqn (S15)–(S17) in Section S5.1).

The MACRO model formulation also includes several additional operational and policy constraints: (1) regional constraints requiring all captured CO_2 to be utilized, transported, or sequestered (Section S5.4), (2) a resource adequacy constraint for the electricity sector that enforces a balance between supply and demand of firm capacity (Table S22); (3) ramping and minimum output constraints for technologies with limited flexibility, such as thermal power generators, fossil based H_2 production, DAC, and fuel production technologies (Table S23); (4) electricity and H_2 storage inventory balance constraints at hourly and weekly scales, described in ref. 46 and 47; and (5) a system-wide CO_2 emissions policy limit (Section S5.5). The complete model implementation and documentation are available in a public GitHub repository,[45] with detailed formulations for liquid and gaseous fuels modeling in Section S5 of the SI.

2.2. Case study description

We used MACRO to investigate future energy systems with net-zero emissions using a nine-zone representation of the contiguous U.S. energy system (Fig. S24). All technologies except electricity generation and transmission, fossil liquids production, and NG production are modeled as greenfield developments, with investment decisions endogenously determined. Projected hourly demand for electricity, as well as annual demands for H_2, liquid fuels (gasoline, jet fuel, diesel, see Fig. 2A) and NG for each region in 2050 were obtained from the low electrification (E^-) demand scenario of the Net-Zero America Study[2] (Table S12). Although this scenario is labeled "low electrification" in the underlying literature source, it still represents a net-zero transition path that includes substantial electrification of end uses, leading to higher electricity demand and lower demand for liquid fuels and NG relative to today. Apart from electricity that is represented with hourly variations, the demand profile for each of the other commodities is represented as constant hourly demand that sums to the annual demand for the entire year.

The choice of 2050 as a model year is primarily motivated by the availability of outputs (*e.g.*, final energy demands) from other studies that can be used as inputs for this study. However, the key findings from this paper related to the drivers of fuel process selection in deeply decarbonized systems are not likely to be sensitive to assumptions about when the net-zero year occurs. Put differently, because we solve for a single future state,

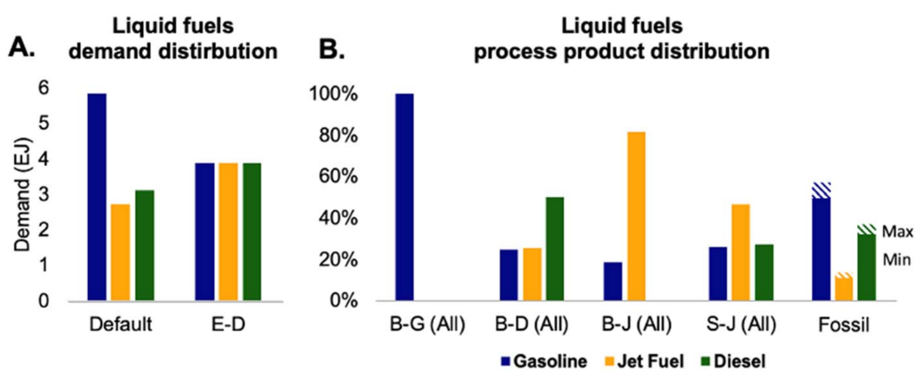

Fig. 2 (A) Liquid fuels demand distributions used in this study for the future net-zero year. The default demand distribution is obtained from Princeton University's Net-Zero America study low electrification scenario as shown in Table S12,[2] and the "E-D" (equal demands of gasoline, jet fuel, and diesel) distribution is obtained by allocating the total default liquid fuels demand equally across the individual liquid fuel products. (B) Fuel product (gasoline, jet fuel, and diesel) distribution of liquid fuel production pathways modeled in this study – see Table 1 for additional process information. For fossil liquids, refinery product slate constraints are highlighted by showing minimum (solid bars) and maximum (dashed bars) values for gasoline, jet fuel, and diesel. Labels refer to whether process is bio ("B") or synthetic ("S"), as well as the dominant fuel product ("G" – gasoline, "J" – jet fuel, "D" – diesel). "All" indicates that the product distribution is independent of CC level.

it is possible to interpret these results as describing a future year in which these final demands and CO_2 emissions are attained, which need not be 2050.

To approximate year-round system operations, the model simulated operations over 26 representative weeks. Of these, 23 were derived using a time-domain reduction method based on *k*-means clustering applied to a single year of hourly energy demand and resource availability time series data for renewable resources (*e.g.*, wind, solar, hydro).[48] In addition, three additional "extreme" weeks corresponding to periods of peak electricity demand and minimum solar and wind availability were included to capture the impact of such operating variations on system capacity decisions. The resulting 26 weeks were sequenced chronologically and weighted to the number of actual weeks represented, allowing for a tractable and accurate approximation of full-year operations.

Cost and performance assumptions for technologies in the electricity, H_2, and CO_2 supply chains are summarized in Section S3.2 of the SI, and mainly follow the assumptions used in a previous study.[23] Annualized CO_2 sequestration rates and associated injection costs were sourced from the National Renewable Energy Laboratory (NREL) Regional Energy Deployment System (ReEDS) model, with annualized rates estimated as the constant yearly injection rate that would fully utilize the available CO_2 storage over a 100 year period (Table S29 and Fig. S25).[49] Biomass supply assumptions were obtained from the 2023 Billion-Ton Report from which regional supply curves were constructed to represent the regional availability and costs of various biomass types – herbaceous, woody, and agricultural residues as shown in Fig. S26–S31 and Tables S38–S39.[50] The average regional energy and carbon content of each biomass category was defined based on the 2023 Billion-Ton Report and primarily GREET 2023 data, respectively (Table S40).[51] The assumed biomass supply, parametrized *via* regional supply curves (see Fig. S26–S31), is available to all biomass conversion pathways in the model, including liquid fuels, electricity, hydrogen, and gaseous fuels. The optimization framework allocates biomass across sectors based on system-wide cost minimization, reflecting the relative value of biomass for emissions reduction and energy supply in each application.

The supply of fossil liquid fuels is assumed to be unconstrained and priced using the national 2050 average fuel cost for the transportation sector projected by the U.S. Energy Information Administration's (EIA) Annual Energy Outlook (AEO) 2023 reference scenario[52] (Table S32). In addition, the product yields of fossil gasoline, jet fuel, and diesel from U.S. refineries from 2009–2023 were used to develop lower and upper bounds on the fossil liquid supply distribution.[43] The implications of refinery flexibility enabled by reconfigurations or new technology are considered in an additional sensitivity case discussed in Section 3.5.

Cost and performance assumptions for biofuel pathways were obtained from various TEAs in the literature (Table S34), each with unique product distribution mixes, as highlighted in Fig. 2B. Modeled biofuels pathways include: (a) biomass gasification followed by methanol synthesis to produce gasoline exclusively (B-G),[21] (b) biomass gasification followed by FT[19] to primarily produce diesel (B-D), along with gasoline and jet fuel as co-products, (c) biomass gasification followed by FT[20] with different CC rates and an alternative product distribution tilted toward jet (B-J) but with some gasoline and electricity production. Including CC variations, a total of nine biofuel processes were represented. Cost and performance assumptions for synthetic liquid fuel production were derived from the TEA study of Zang *et al.*,[22] which considers one process with and without CC, namely H_2 and CO_2 conversion to liquids using FT technology that produces a mix of gasoline, jet fuel, and diesel (S-J) described further in Table S33. In this study, capital and operating costs (other than feedstock costs) are assumed to be scenario independent. While capital costs may decline with deployment in real markets, this interaction is challenging to represent explicitly, so as an alternative, we consider a sensitivity to capital costs in Section 3.6.

The supply of fossil NG is also assumed to be unconstrained and available at the average delivered price in EIA's AEO 2023 reference scenario. Synthetic and biomass-derived NG pathways are parametrized using available literature (see Tables S36 and S37 for details). Cost and performance assumptions for synthetic NG production are based on a TEA study of CO_2 methanation process,[53] while bio-NG production assumptions are based on a TEA study of a process utilizing gasification to produce syngas followed by fermentation to produce NG.[54] All cost parameters in this study are standardized to 2022 dollars to account for differences in dollar-years between various references.

For biomass and synthetic fuel pathways not originally modeled with CO_2 capture, we developed alternative process variants with different capture rates using an approximation method discussed in Section S2.2, thereby ensuring that each fuel pathway includes configurations spanning a range of CC rates (Table 1). This method involves matching the CO_2 concentrations of the flue gas stream(s) in each pathway to analogous industrial point sources (*e.g.*, flue gas in cement or ethanol production) and applying the corresponding capture costs and energy requirements reported in published techno-economic assessments (TEAs) of industrial point-source CO_2 capture.[55,56] This approach omits pathway-specific energy integration opportunities and could be viewed as a conservative estimate of energy impacts of CC implementation. Detailed costs, energy requirements, and performance assumptions for all CO_2 capture variants are provided in Tables S33 and S34, with detailed carbon balances shown in Fig. S32–S35 of the SI.

In addition, energy and carbon balances of the various pathways are harmonized as described in Section S2.3. This harmonization allows for the application of user-defined carbon content for biomass and fuels in the MACRO model, while preserving the energy conversion and product distribution as reported in the respective process-level TEAs.

2.3. Scenarios

We evaluated systems with net-zero emissions, varying assumptions about biomass and CO_2 sequestration resource availabilities as shown in Fig. 3A. Tighter constraints on these

Table 1 Key performance and assumptions of alternative liquid fuels production pathways in this study: reported biofuel parameters are based on weighted average value of 47.3% carbon content per biomass weight and 18.15 MMBtu per tonne biomass from the high mature market scenario of the 2023 Billion-Ton Report.[50] Levelized capex + opex cost contribution refers to *n*th-of-a-kind facilities and includes fixed and all variable operating costs except those related to energy and feedstock inputs. For pathways not originally modeled with CO_2 capture, capture variants were developed using the approximation method described in Section S2.2 in the SI. Energy contents are reported in higher heating value (HHV). Carbon conversion = carbon content of fuel products divided by the carbon content of the feedstock. Carbon conversion is not a technology input parameter in the MACRO model. Instead, biofuel production technologies are modeled using energy conversion efficiency and product distribution inputs as described in Section S5.1 of the SI (see eqn (S8)–(S10)). As such, the actual carbon conversion might differ according to the type of biomass consumed as shown in Tables S38 and S39. Detailed input assumptions of the pathways are shown in Tables S33 and S34, with carbon balances shown in Fig. S32–S35 of the SI. Process labels refer to whether process is bio ("B") or synthetic ("S"), the dominant fuel product ("G" – gasoline, "J" – jet fuel, "D" – diesel) as shown in Fig. 2B, and the rate of CO_2 capture ("CCXX") if applicable. "R" in S-J-CC99-R refers to a variant whereby the capture CO_2 is recycled back to the input CO_2 feed, thus increasing the carbon conversion

Process	B-G	B-G-CC31	B-G-CC99	B-J-CC75	B-J-CC84	B-J-CC99	B-D	B-D-CC53	B-D-CC99	S-J	S-J-CC99	S-J-CC99-R
Carbon conversion (%)	28.3	28.3	28.3	24.3	32.0	24.3	38.2	38.2	38.2	47.2	47.2	98.9
CO_2 capture rate (%)	—	31.0	99.3	74.8	83.9	99.0	—	52.8	99.5	—	99.0	—
Levelized capex + opex contribution ($ per GJ_{fuels})	14.21	17.03	21.87	30.57	23.91	32.62	13.67	15.14	17.41	10.93	13.83	13.83
Biomass input ($GJ_{biomass}$ per GJ_{fuels})	2.64	2.64	2.64	3.10	2.36	3.10	1.98	1.98	1.98	—	—	—
Electricity input (GJ_e per GJ_{fuels})	—	0.05	0.57	—	—	—	1.07	1.10	1.34	0.02	0.33	0.33
H_2 input (GJ_{H_2} per GJ_{fuels})	—	—	—	—	—	—	—	—	—	1.92	1.92	1.92
CO_2 input (tonne per GJ_{fuels})	—	—	—	—	—	—	—	—	—	0.14	0.14	0.07
Approximation method for CO_2 capture	—	Yes	Yes	CO_2 capture present in original reference			—	Yes	Yes	—	Yes	Yes
References	21			20			19			22		

resources do not necessarily need to be interpreted as physical resource constraints but could represent preferences expressed through other forms of policy that restrict availability. The low (LB: 9.5 EJ per year) and high (HB: 15.9 EJ per year) biomass availability scenarios are based on the supply curves for low and high mature market, respectively, from the 2023 Billion-Ton Report.[50] The low (LS: 433 $MtCO_2$ per year) and high (HS: 866 $MtCO_2$ per year) availability scenarios for CO_2 sequestration assume that 5% and 10%, respectively, of the CO_2 sequestration capacity at each site included in the NREL ReEDS model is available.[49] The 10% limit is based on suggestions in the literature that around 10% of CO_2 sequestration sites in the U.S. may be economically viable.[57]

For each of the above scenarios, we also evaluated cases with varying assumptions about fuel technology product flexibility as shown in Fig. 3B. "FF" and "PF" refer to scenarios with full

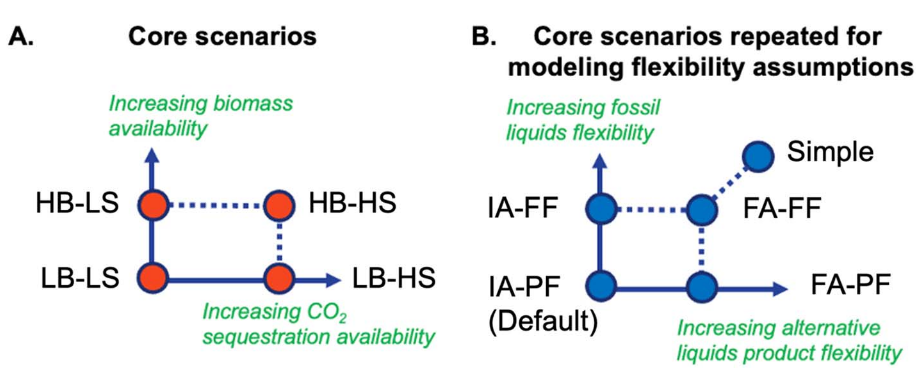

Fig. 3 (A) Scenario matrix showing four core scenarios assessed in this study by varying assumptions about biomass and CO_2 sequestration resource availability. "HB" = high biomass of 15.9 EJ per year, "LB" = low biomass of 9.5 EJ per year, "HS" = high CO_2 sequestration of 866 Mt CO_2 per year, "LS" = low CO_2 sequestration of 433 Mt CO_2 per year. All scenarios assume a net-zero emissions constraint. (B) Matrix of liquid fuels modeling flexibility in which the four core scenarios in (A) are rerun with other assumptions about fossil liquid fuels and alternative liquid fuels supply flexibility. "IA" = Inflexible alternative liquid fuels where liquid fuel product slate strictly follows the original product distribution of their respective literature references. "FA" = Fully flexible alternative liquid fuels where the fuel product slate of each technology is allowed to vary while respecting total liquid fuel output (on an energy basis) reported by the literature reference. "PF" = partially flexible fossil liquid fuels where the ratio of purchased conventional fossil gasoline, jet fuel, and diesel lies within historical bounds of U.S. fossil petroleum refineries.[43] "FF" = Fully flexible fossil liquid fuels where conventional fossil gasoline, jet fuel, and diesel can be produced in any ratios. "Simple" = Simplified modeling assumptions of liquid fuels without any product differentiation of gasoline, jet fuel, and diesel, with aggregated liquid fuels demand and weighted average conventional fossil liquid fuels purchase price and emission factors. The "IA-PF" modeling assumption is used as the default in this study.

flexibility and partial flexibility in fuel product distribution from fossil liquids supply, respectively. Here partial flexibility refers to the product distributions that are constrained by historical refinery product distributions. Similarly, "FA" and "IA" refer to scenarios with full flexibility and no flexibility, respectively in product distribution from each alternative fuel production technology. In effect, under "FA", we assume that the processes can produce the product distribution with greatest system value without any additional costs (see Section S5.2 for formulation), while under "IA", the product distribution of each process is restricted to the distributions reported in the original literature sources (seen in Fig. 2B). We also evaluate an additional case, termed "simple model", without any fuel product differentiation in demand or supply, to quantify the impacts of simplifying liquid fuels modeling assumptions, given the prevalence of this approach in coarser-resolution models. The "IA-PF" scenario is used as the base case representation of fuels supply product flexibility. We also undertake additional sensitivity analysis to

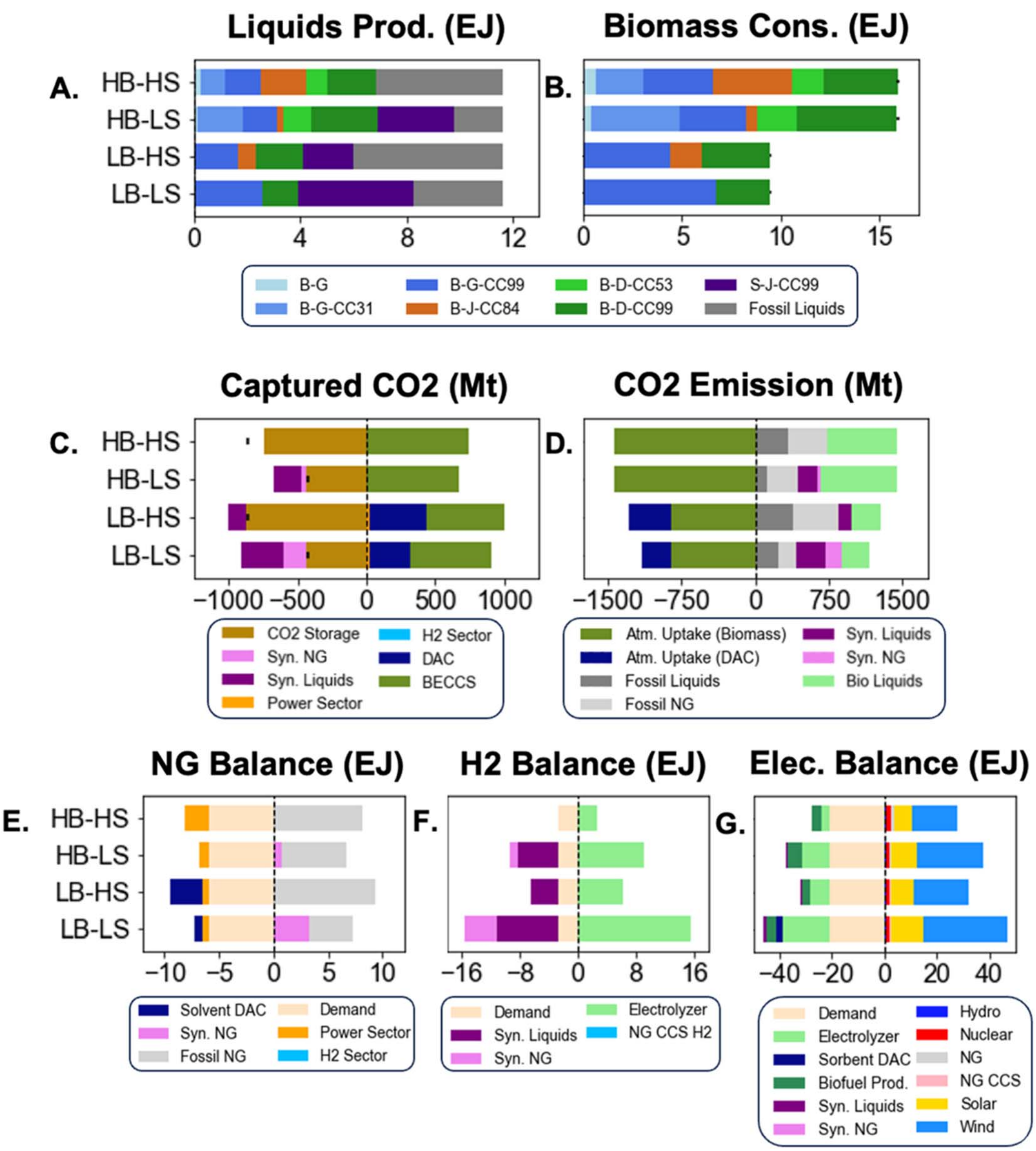

Fig. 4 Energy system impact of varying biomass and CO_2 sequestration availability in the net-zero year. These cases use default "IA-PF" modeling assumptions described in Fig. 3B and default demand distribution described in Fig. 2A; (A) total liquid fuels production by technologies, (B) biomass consumption by technologies, (C) captured CO_2 balance, (D) CO_2 emission balance, (E) natural gas balance, (F) H_2 balance, (G) electricity balance. Liquid fuels production technology labels follow Table 1. "DAC" = direct air capture, "BECCS" = bioenergy with CO_2 capture and sequestration, "NG" = natural gas, "CCS" = CO_2 capture and sequestration. The resource limits for biomass and CO_2 sequestration are indicated by the bars in (B) and (C) respectively. In each panel for marketable commodities, positive values indicate production, and negative values indicate consumption. "Demand" indicates exogenously assumed final demand. For CO_2 emissions, positive values indicate combustion emissions, while negative values indicate atmospheric uptake. "Atm. uptake (biomass)" and "Atm. uptake (DAC)" refer to the carbon content of the biomass resource and CO_2 removal by DAC processes, respectively. The contributions from different liquid production technologies to each liquid fuel product demand are shown in Fig. S1.

consider alternative assumptions about liquid fuel demand distributions and capital costs of alternative fuel production technologies.

3. Results

3.1. Energy system impacts of biomass and CO_2 storage availability

Fig. 4 summarizes the energy system impact of varying biomass and CO_2 sequestration availability in the base case ("IA-PF" in Fig. 3B), which assumes a constrained fuel product distribution from each fuel production pathway. In all scenarios, biomass is fully utilized to produce liquid fuels, indicating that biomass used for fuels outcompetes the use of biomass in other sectors as explained further below. Biofuels account for 59% of total liquid fuels in high biomass (HB) scenarios and 34–35% in low biomass (LB) scenarios. As the product slates of both alternative and fossil fuel pathways are constrained, multiple biofuel pathways are deployed, providing the fuel specific products needed to exactly match the specified fuel demand distribution.

Biofuel deployment also enables the use of fossil liquid fuels when paired with CCS, as the sequestered biogenic CO_2 provides removals that offset fossil emissions (Fig. 4C and D). Accordingly, for the same biomass resource availability, the HS scenario enables more fossil fuel use compared to the LS scenario (41% *vs.* 16% of total demand in HB, and 49% *vs.* 30% in LB scenarios). Conversely, when sequestration is more constrained, synthetic fuel production increases (from 0% to 25% of fuel demand in HB, and from 16% to 38% in LB scenarios). Constraining biomass resource availability limits the amount of biofuel that can be produced, with the remaining fuel demand supplied by fossil fuels, if the assumed CO_2 sequestration availability allows for it, and synthetic fuel production. These results indicate a tendency for liquids production in highly decarbonized systems to rely on both fossil fuels (when removals can offset remaining emissions) and biofuels, with synthetic fuels deploying only when biomass availability is constrained (which limits biofuel production) or when CO_2 sequestration availability is constrained (which limits fossil liquid production by limiting removal potential). It is worth noting that synthetic fuels can be produced from biogenic CO_2 (*e.g.*, CO_2 captured from biofuel production), which could be interpreted as biofuel produced from an intensified process in which more of the carbon from primary biomass is converted to fuel.

The optimal carbon capture (CC) rate across the biofuel pathways is primarily affected by the biomass resource assumption, as seen by the reliance on processes with higher CC rates in the LB scenarios than in the HB scenarios. Higher CC rates are consistent with higher marginal CO_2 abatement costs in LB ($549–664 per tonne) compared to HB ($119–299 per tonne) scenarios (see Table S1). These carbon prices are also consistent with the observation that DAC only deploys in the LB scenarios (see Fig. 4D) in which biomass cannot provide the amount of atmospheric carbon required for CDR or utilization. Furthermore, the availability of CO_2 sequestration impacts the choice of DAC technologies – only the lower cost natural gas-driven solvent-based DAC pathway gets deployed under the HS scenario, while under the LS scenario with higher CO_2 abatement costs, we also see deployment of the more expensive sorbent-based, electricity-powered DAC pathway, which requires less CO_2 sequestration per tonne CO_2 removed.

In the NG production sector (Fig. 4E), there is no deployment of biomass-based NG, with fossil NG dominating supply and synthetic NG production sensitive to CO_2 sequestration availability (0% in HS *vs.* 11–45% in LS scenarios). Greater deployment of biofuels in the liquid fuels sector relative to the NG sector is driven in part by differences in abatement costs between the biomass technologies in the two sectors. Compared to fossil liquids, fossil NG is less expensive ($4.89–8.85 per MMBtu *vs.* $22.18–28.53 per MMBtu) and has a lower CO_2 emission factor (5.4 *vs.* 7.2–7.3 kg CO_2 per MMBtu) (Tables S30, S31 and S35). Hence, biomass use in the liquid fuels sector delivers greater emissions reduction for a given increase in cost relative to the incumbent fossil technology.

Across the scenarios, electrolytic H_2 dominates production. Prior work suggests that the choice between electrolytic and natural gas-based hydrogen production depends in part on infrastructure and flexibility assumptions.[22] In addition, constraints on CO_2 storage increase the cost of options that require carbon capture and sequestration. Regardless of the type of hydrogen produced, the magnitude of H_2 production is substantially affected by deployment of synthetic fuels. For instance, H_2 production in the LB-LS scenario, with the most synthetic fuel production, is about five times exogenous H_2 demand. The strong power-H_2 sector coupling due to electrolyzer deployment in these cases also causes electricity generation to increase with increasing synthetic fuel production. Within the power sector, VRE accounts for 86–95% of total electricity generation, with the balance provided by a combination of other resources, including nuclear, hydro and unabated natural gas capacity dispatched infrequently (2–6% utilization). This result is consistent with other net-zero studies of the electric power sector showing that substantial unabated natural gas capacity remains in the system mainly as low-utilization firm capacity, with VRE providing the most electricity generation.[58] Overall, the energy system results illustrate how biofuel, fossil fuel, and synthetic fuel shares are affected by biomass and CO_2 sequestration assumptions, as well as how the overall energy system responds.

3.2. Disposition of atmospheric carbon

Two metrics summarize the main differences in fuels technology deployment across the various scenarios in Fig. 4: (a) the disposition of carbon emissions from biofuel production – either emitted or captured (Fig. 5A) and (b) the disposition of captured atmospheric carbon, which can be either converted to fuel, *i.e.*, utilized, or sequestered (Fig. 5B).

Across scenarios, biomass availability emerges as the primary factor affecting the share of atmospheric carbon that is re-emitted, which is effectively determined by endogenously choosing the CO_2 capture rates for the different biofuel technologies. Under constrained biomass availability in the LB

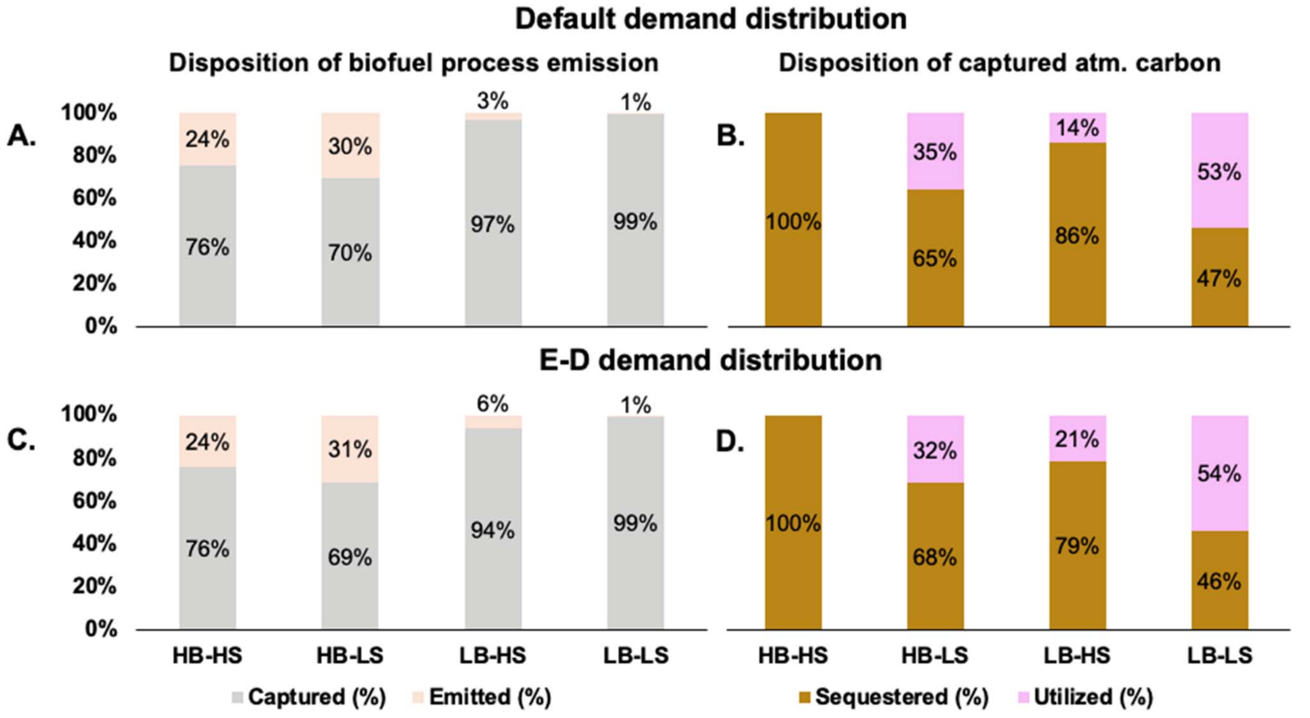

Fig. 5 (A and C) Disposition of biofuel production carbon emissions (excludes the carbon content in biofuel products), (B and D) disposition of captured atmospheric carbon from biofuel processes and direct air capture across the core scenarios described in Fig. 3A for default "IA-PF" modeling assumptions as described in Fig. 3B, under default (panel A and B) and "E-D" (panel C and D) demand distributions as described in Fig. 2A. Emitted = carbon vented (*i.e.*, not captured) in biofuel production processes, sequestered = captured atmospheric carbon that is sequestered in geological storage, utilized = captured atmospheric carbon that is utilized for synthetic fuels production (both liquid fuels and NG).

scenarios, system-level biofuel CC rates are 97–99% (Fig. 5A), whereas in the HB scenarios, the system level biofuel CC rates are lower at 70–76%. For a given amount of remaining fossil liquids, lower biomass resource availability implies that more of the biogenic carbon must be captured and sequestered to offset fossil emissions. This incentive to increase biogenic CO_2 capture further increases in scenarios with lower biomass availability because these scenarios tend to also have more remaining fossil liquids than scenarios with higher biomass availability, all else equal. The tendency toward higher carbon capture rates when biomass is limited is consistent with the higher observed carbon prices in these runs, which would support the additional cost of higher capture rates (Table S1).

Whereas biomass availability drives the biofuel process CC rates, the availability of CO_2 sequestration resources largely determines the disposition of captured atmospheric CO_2 between sequestration or utilization. It is worth noting that atmospheric carbon can come from combusting or processing biomass or from DAC, with the latter only deployed under LB scenarios, contributing 26–33% of total atmospheric CO_2 uptake. In LS scenarios, 35–53% of captured CO_2 is utilized for fuel production, whereas in the HS scenarios, 0–14% of captured CO_2 is used for fuel production (Fig. 5B). This increased coupling between biofuel and synthetic fuel production in the LS scenarios effectively creates a combined bio-synthetic fuel pathway with atmospheric carbon (including biogenic CO_2) conversion to fuel of 49–63% under the LS scenario as compared to 32–33% in the HS scenario (Table S2). When biogenic CO_2 from biofuel production is captured and used to produce more synthetic fuel, this combination could alternatively be viewed as a single intensified biofuel production pathway.

3.3. Economic drivers of fuel pathway selection

To assess differences in the deployment of individual liquid fuel technologies across scenarios, we evaluate their levelized production costs ($/GJ) and compare them with the system-level average prices of fuels in each scenario (Fig. 6). The levelized production cost includes: (a) scenario-dependent costs, such as the cost of energy and other inputs for each technology, which are estimated based on their scenario-dependent system-average shadow prices (*i.e.*, dual variables of commodity supply-demand balances averaged over regions and time) (see eqn (S2)–(S4) in Section S2.1), and (b) scenario-independent costs such as capital costs (CAPEX) as well as fixed and variable operation and maintenance costs (FOM and VOM) that are also used to parameterize technologies in the CEM.

Fig. 6 highlights how the absolute levelized production cost of alternative fuel technologies is impacted more by scenario-dependent costs, reflecting resource availability assumptions, rather than scenario-independent, technology specific factors such as capital cost and non-energy, non-feed operating costs, which are generally the focus of most TEA studies. For example, the cost of biofuel technologies producing gasoline *via* MeOH

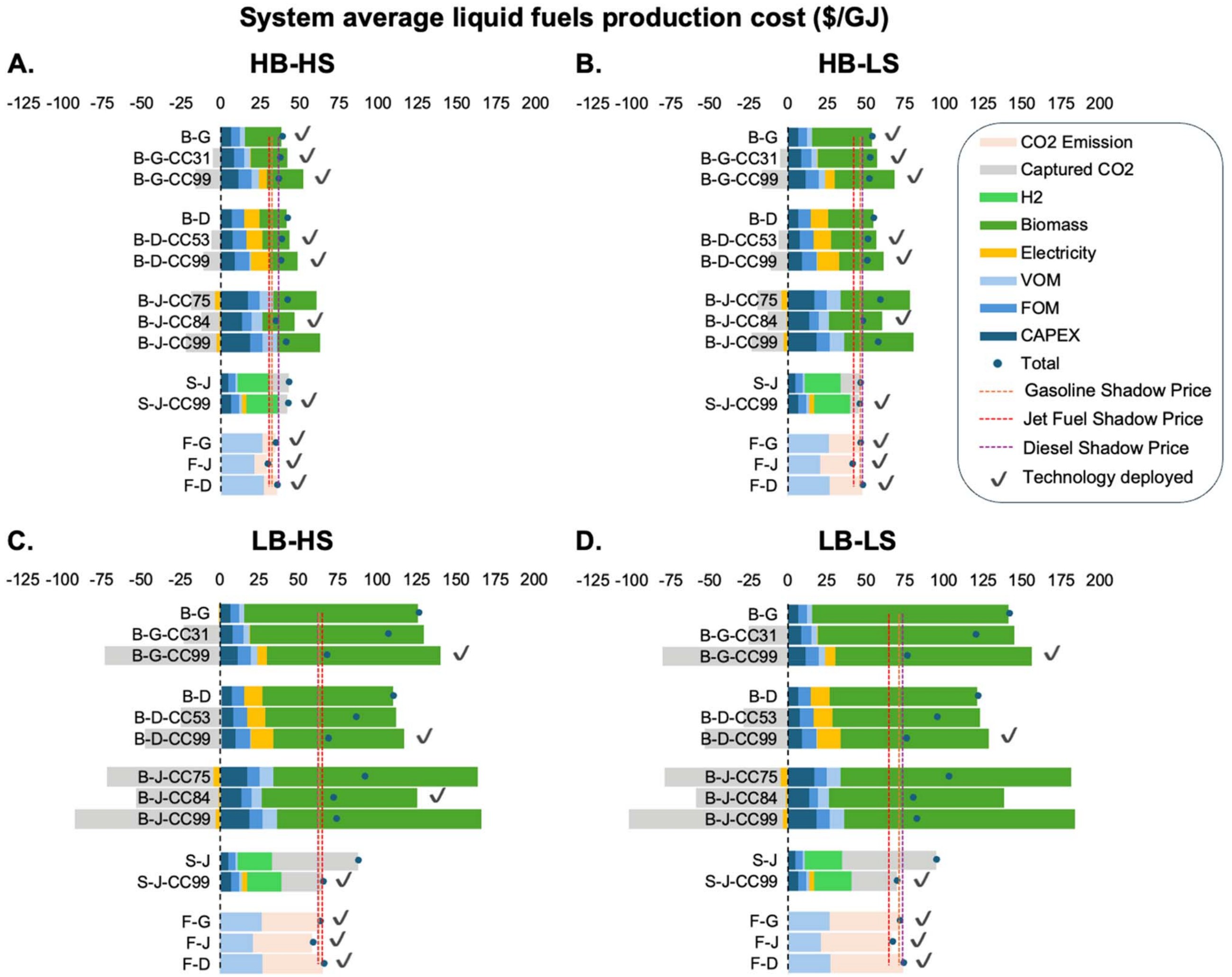

Fig. 6 System-level average production costs of liquid fuel pathways across core scenarios described in Fig. 3A for default "IA-PF" (Inflexible alternative liquid fuels with partially flexible fossil liquid fuels) modeling assumptions described in Fig. 3B. The stacked bars show the average cost per unit of fuel ($ per GJ) for each technology in Table 1, with product distribution shown in Fig. 2B. Scenario-dependent costs for biomass, electricity, hydrogen, and captured CO_2 are calculated using system-averaged time-weighted values according to eqn (S2)–(S4) in Section 2.1 of the SI. These values are based on the shadow prices for each commodity supply-demand balance for a given scenario. Additional costs, such as capital costs (CAPEX), fixed operating and maintenance (FOM) costs, and variable operating and maintenance (VOM) costs, are model input assumptions. The vertical dashed lines represent the system-average shadow prices for gasoline, jet fuel, and diesel. Since deployment decisions occur at the regional level, and the figure uses system-averaged prices to report scenario-dependent costs, the estimated cost of each deployed technology may not exactly equal fuel revenue.

with 99% CC varies by more than 2× ($36.5 per GJ *vs.* $76.3 per GJ), across the scenarios, while its scenario-independent costs only amount to $24.1 per GJ. In the case of synthetic fuels, although H_2 is a major cost component, as noted by various TEA studies, we find that its contribution is comparable to the cost of captured CO_2 in two of three scenarios with synthetic fuels deployment (LB-LS in Fig. 6D, and LB-HS in Fig. 6C). We also note that correlations between commodity shadow prices, which are generally not considered in TEA studies, play an important role in setting the levelized production cost of individual technologies. For instance, even though biomass prices are 3–4× greater in LB than in HB scenarios (Fig. S5), these increased costs are partly offset by increased revenue from CO_2 capture due to the higher carbon prices (*i.e.*, CO_2 abatement costs – see Table S1) associated with these scenarios.

Besides showing absolute levelized costs, Fig. 6 also highlights relative differences in costs among different technologies. Notably, when carbon prices are relatively low, such as in the HB-HS scenario (Fig. 6A), differences among system-average levelized costs of biofuel pathways with different CO_2 capture rates are relatively small. In this case, regional differences in costs play a more prominent role in driving technology adoption. For example, in regions with limited CO_2 storage capacity such as in the Northeast and Mid-Atlantic, the system adopts lower CC pathways to avoid investment in CO_2 pipelines to transport captured CO_2 to neighboring regions. On the other hand, where CO_2 storage is available locally such as in the North-Central U.S., higher CC pathways are adopted.

3.4. Sensitivity to liquid fuel demand distribution

Given uncertainty in demands for different fuel products, we examine the robustness of the system outcomes to alternative assumptions regarding the liquid fuels demand distribution. Changing the fuel demand distribution could impact the fuel production mix, particularly under the scenario in which the fuel product distribution of each technology is constrained, as is true in our base case ("IA-PF"). We tested this hypothesis by considering an alternative equal fuel demand distribution ("E-D") case in which demand for gasoline, jet, and diesel is equal rather than dominated by gasoline as in the base case (Fig. 2A).

This alternative demand scenario is motivated by economy-wide trends related to growing aviation and freight demand (increasing jet and diesel fuel demands, respectively) and electrification of light-duty vehicles (declining gasoline demand). The E-D case is evaluated to represent a possible future fuel demand scenario with a lower contribution from gasoline, with total liquid fuel demand held constant to isolate the effect of demand composition. As such, it should be interpreted as a robustness test rather than a projection tied to a specific electrification rate.

Fig. 7A–D present the resulting liquid fuel production mix, along with broader system outcomes including electricity, H_2, and NG production. We find that key system outcomes identified previously such as the deployment of high CC biofuel pathways in LB scenarios, and the increased reliance on synthetic fuels under constrained CO_2 sequestration resources in LS scenarios remain largely unchanged. Likewise, the two summary metrics identified earlier – disposition of biofuel process emissions and disposition of captured atmospheric carbon – follow the same patterns observed in the base case fuel demand scenario (Fig. 5C and D). This consistency underscores the dominance of resource constraints (which may reflect physical resource constraints or policy preferences) rather than fuel demand distributions in determining the optimal system deployment of biofuels, synthetic fuels, and fossil fuels.

While fuel demand distributions have a modest impact on the relative deployment of biofuels, fossil fuels, and synthetic fuels, they have a greater impact on the competition among biofuel production technologies. In the default demand scenario, gasoline-dominated (B-G) biofuel pathways contribute a significant share of liquid fuels production, with gasoline accounting for 50–74% of biofuels (Fig. S4). On the other hand, the share of gasoline in biofuels decreases to 22–32% in the E-D scenarios (Fig. S4), as the system shifts toward diesel and jet-dominated (B-D and B-J) biofuel processes. This reallocation reflects the flexibility of the biofuel portfolio to adjust output mixes to align with changes in demand distributions. In contrast, the flexibility of fossil liquid supply is restricted by historical refinery yield constraints that favor a gasoline-heavy product distribution (see Fig. 2B). The historical refinery product mix aligns well with the base case fuel demand

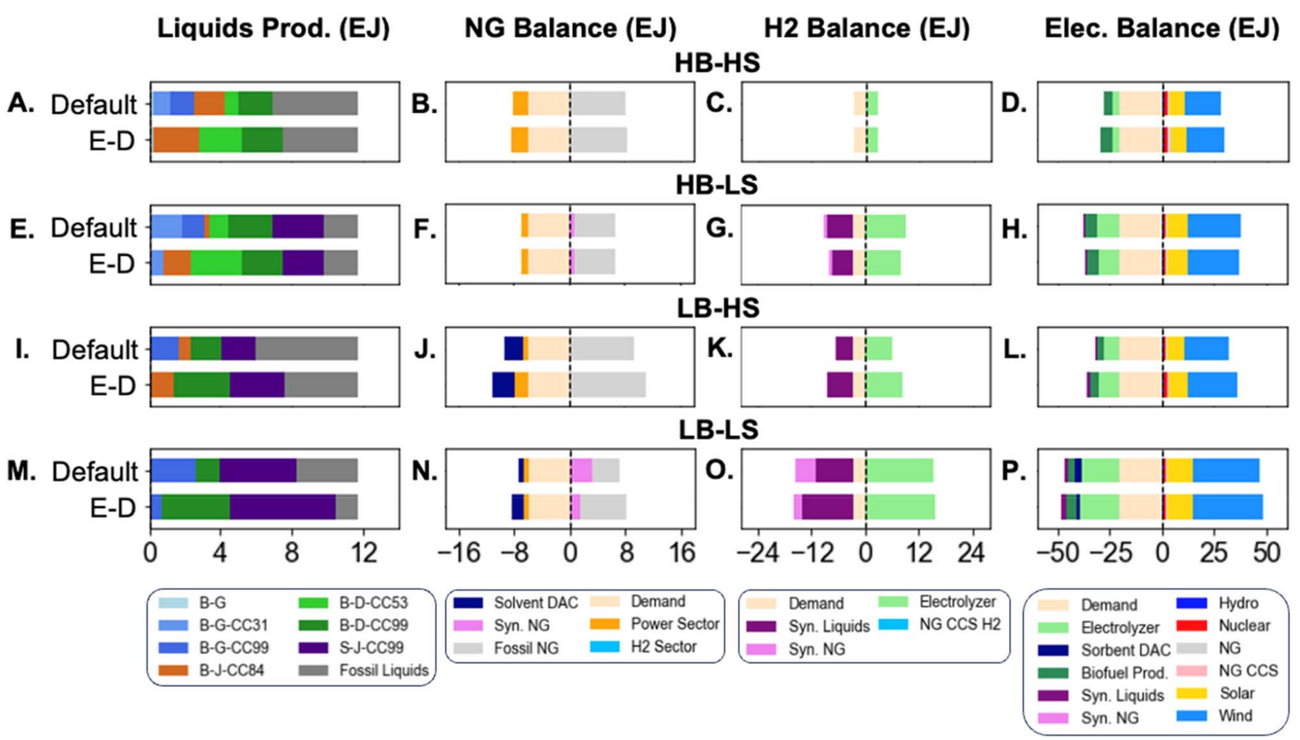

Fig. 7 Impacts of fuel demand distribution on energy system outcomes: liquid fuels production by pathway (panels A, E, I and M), NG balance (panels B, F, J and N), H_2 balance (panels C, G, K and O), and electricity balance (panels D, H, L and P) across core scenarios described in Fig. 3A for "IA-PF" modeling assumptions described in Fig. 3B. The scenarios are evaluated under the default and "E-D" demand distributions described in Fig. 2A. Liquid fuels production technology labels follow Table 1. The contributions from different liquid production technologies to each liquid fuel product demand are shown in Fig. S3.

distribution, especially under LB scenarios with increased reliance on fossil and synthetic fuels. However, when demands are assumed to shift, as in the E-D scenarios, fossil refinery yields no longer match the demand distribution, and the share of fossil liquid supply decreases by 4–18% across the core scenarios.

When biomass resource availability is high, the model deploys a mix of biofuel processes that produces an optimal distribution of gasoline, jet, and diesel such that the remaining liquid fuels demand can be fulfilled with the least-cost mix of fossil and synthetic fuels. Therefore, the proportion of total bio, synthetic, and fossil liquid fuels under the base and E-D demand distributions are similar in the HB scenarios. However, under constrained biomass availability, the ability to optimize product distribution through biofuel process selection is more limited. Combined with the limited flexibility of fossil liquid fuels, more synthetic liquid fuels fulfill the demand distributions that are less gasoline-heavy (Fig. 7I and M).

3.5. Sensitivity to liquid fuels supply flexibility

To assess the robustness of energy system outcomes to modeling assumptions about liquid fuel technology product supply flexibility, we simulated the core matrix under four alternative sets of assumptions about production flexibility, as described in Section 2.3 and shown in Fig. 3B. These cases span a range of possible ways to represent liquid fuels in energy system models and enable us to assess how product distribution constraints affect process selection and system-level decarbonization outcomes. In particular, the FF cases allow refineries to vary the fuel production mix without restriction, and the FA cases allow alternative liquid production technologies to do the same thing.

Fig. 8 illustrates the resulting liquid fuel production mix and key system-wide energy balances across these flexibility assumptions for the core scenarios of biomass and CO_2 sequestration assumptions (Fig. 3A). Overall, we find that the total mix of bio, synthetic, and fossil liquid fuels as well as broader energy system outcomes are similar across the flexibility cases. In other words, key findings driven by biomass availability and CO_2 sequestration limits are mostly unaffected by modeling choices regarding flexibility of liquid fuels processes. Nonetheless, the extent of flexibility can affect process-level deployment decisions. Under fully flexible alternative fuels configurations, process selection is guided

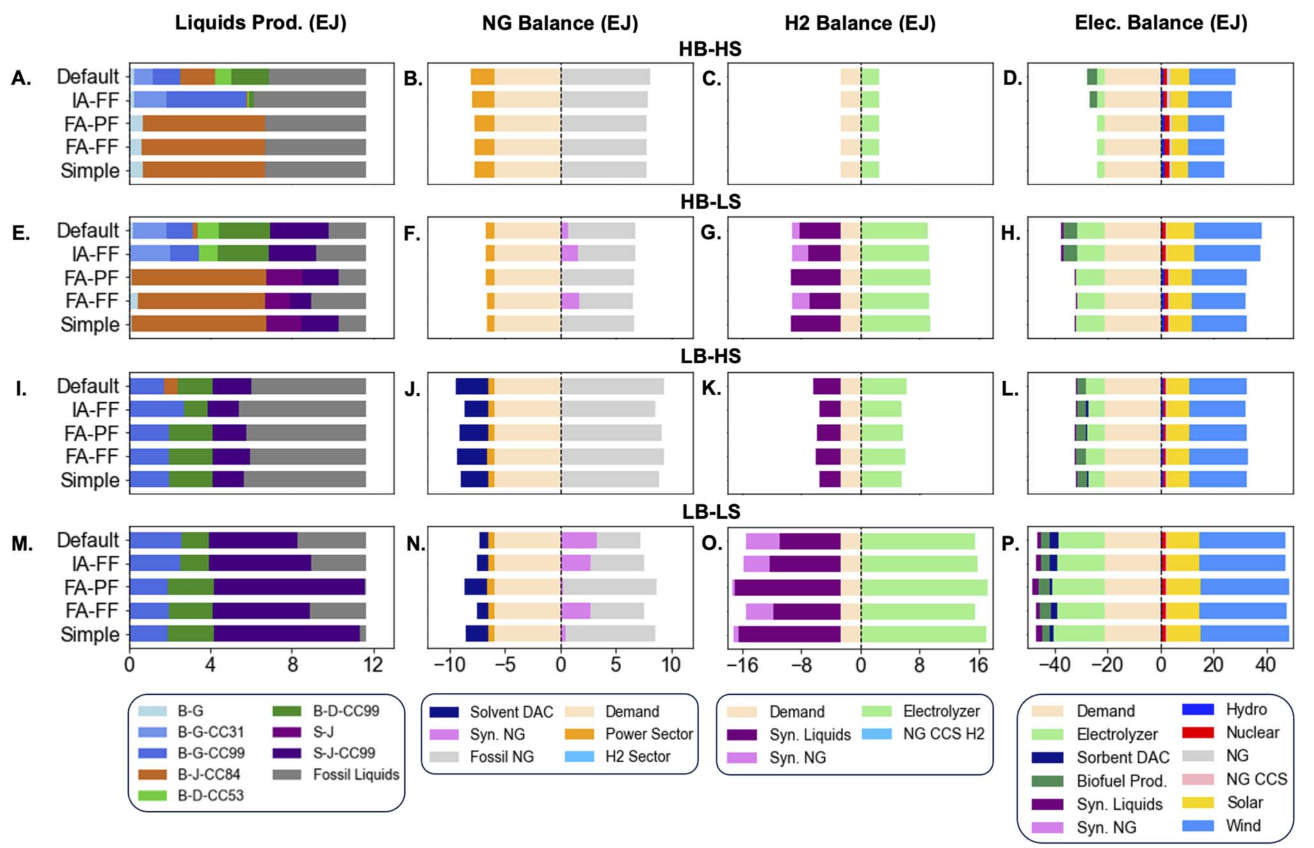

Fig. 8 Effect of liquid fuel flexibility modeling assumptions on energy system outcomes: liquid fuels production by pathway (panels A, E, I and M), NG balance (panels B, F, J and N), H_2 balance (Panels C, G, K and O), and electricity balance (panels D, H, L and P) across the core scenarios described in Fig. 3A, under the default demand distribution described in Fig. 2A. Each row compares the five flexibility modeling assumptions described in Fig. 3B. Default: "IA-PF": inflexible alternative and partially flexible fossil fuels, which is the default assumption used in this study, "IA-FF": inflexible alternative fuels with fully flexible fossil fuels, "FA-PF": fully flexible alternative fuels with partially flexible fossil fuels, "FA-FF": fully flexible alternative and fossil fuels, "Simple": aggregated liquid fuels with no product differentiation. Liquid fuels production technology labels follow Table 1.

primarily by raw production costs as the processes can freely adjust product outputs to match the required demand distribution. In these cases, biofuel technologies are deployed for their cost competitiveness and not limited by their native product distributions.

However, when alternative fuels production flexibility is restricted in IA-FF and IA-PF cases, liquid fuels deployment reflects both process economics and compatibility with the assumed demand profile. For example, in IA-FF, biofuels are allocated mainly to gasoline to satisfy the high gasoline demand, while fossil liquid fuels are mainly in the form of jet fuel due to lower assumed costs. In contrast, the base case (IA-PF) requires all technologies to adhere to their predefined product yields, resulting in a diversified mix of bio, synthetic, and fossil pathways to balance demand across liquid fuel types. Across flexibility variants, we find that outcomes related to the disposition of carbon (see Fig. S10) such as increased biogenic CO_2 venting in HB cases and increased utilization of captured CO_2 in LS scenarios are preserved. Similarly, repeating the alternative modeling flexibility cases with the E-D liquid fuels demand distribution produced comparable outcomes in system-wide energy system results and carbon disposition trends (see Fig. S13–S17). This consistency suggests that key system-level results are driven by biomass and CO_2 sequestration constraints rather than assumptions about liquid fuels production flexibility.

3.6. Sensitivity to alternative liquid fuel capital cost assumptions

To evaluate the robustness of system outcomes to economic assumptions for alternative liquid fuel production pathways, we simulated two alternative capital costs scenarios in addition to the base case: (1) 2x-CAPEX: doubled capital costs for alternative liquid fuel technologies, and (2) 3x-CAPEX: tripled capital costs for alternative liquid fuel technologies. Many literature estimates are developed for *N*th-of-a-kind projects, with initial costs often substantially higher. Therefore, higher capex assumptions could reflect a world in which costs stay higher for longer despite deployment, whereas lower capex assumptions could reflect a world in which technologies reach the assumed costs of mature plants by the net-zero year examined here.

System-level findings remain largely consistent across scenarios for various capital cost assumptions (see Fig. 9), with deployment of processes with higher CO_2 capture rates in LB scenarios, and increased synthetic fuel production in LS scenarios. However, there are some shifts in the disposition of biomass and utilized CO_2 as capital costs are varied. For example, synthetic fuel production shifts from liquid fuels towards NG (Fig. 9E and F) under higher liquids capex assumptions, reflecting the lower abatement costs associated with displacing NG when the cost of alternative liquids

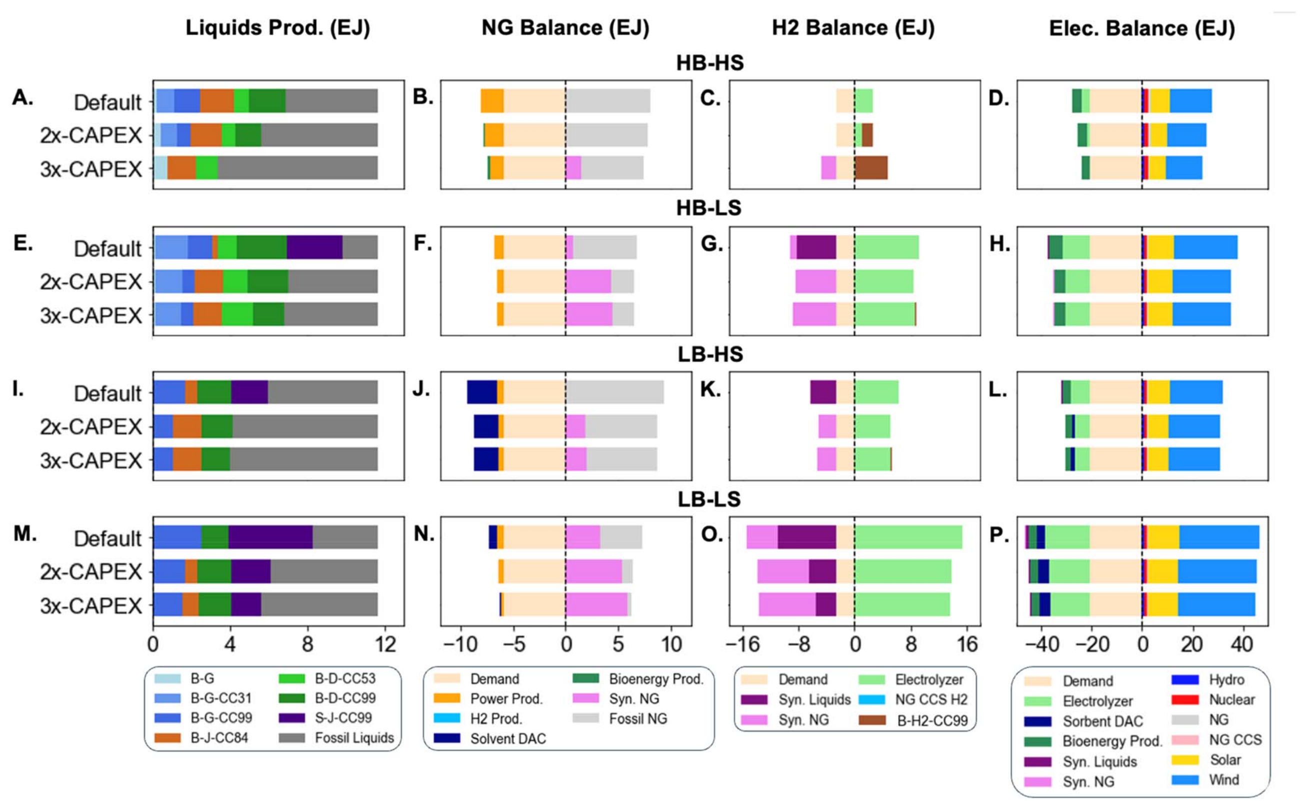

Fig. 9 Energy system outcomes: liquid fuels production by pathway (panels A, E, I and M), NG balance (panels B, F, J and N), H_2 balance (panels C, G, K and O), and electricity balance (panels D, H, L and P) across various capital cost assumptions across core scenarios as described in Fig. 3A for "IA-PF" modeling assumptions as described in Fig. 3B under default demand distribution as described in Fig. 2A. Liquid fuels production technology labels follow Table 1. "2×-CAPEX" = Doubled capital costs for bio and synthetic liquid fuels production technologies, "3×-CAPEX" = Tripled capital costs for bio and synthetic liquid fuels production technologies.

increases. Nonetheless, the share of captured carbon utilized for synthetic pathways (both liquid fuels and NG) remains similar to the default case (see Fig. S21). Similarly, as the capital cost of liquid fuel production increases, biomass use shifts from liquid fuels to hydrogen production in the HB-HS scenario. Since BECCS-H_2 requires a larger biomass input per unit of energy produced compared to biofuels, we do not observe its deployment in scenarios with constrained biomass and CO_2 availability, in which biomass prices are higher than in the HB-HS scenario. Overall, the carbon disposition trends (see Fig. S21) remain similar across scenarios, indicating that assumptions regarding biomass and CO_2 sequestration continue to drive system decisions.

4. Discussion

4.1. Insights relevant to energy system decarbonization

Our analysis highlights that resource constraints, namely biomass availability and CO_2 sequestration, are key drivers of the competition between biofuel, fossil liquid fuel, and synthetic liquid fuel pathways in deeply decarbonized energy systems. While biomass availability generally determines the optimal level of CO_2 capture for biofuel production, the availability of CO_2 sequestration primarily affects the choice between fossil and alternative liquid fuels. We also find that biomass tends to be allocated to liquid fuel production, as its use in other sectors (*e.g.*, hydrogen) emerges only when biofuel process capital costs are substantially higher than default assumptions, and even then, only under the most resource-abundant scenario (HB-HS). This result suggests that the abatement cost of BECCS in liquid fuels is lower than the abatement cost of BECCS in other sectors under the assumptions used in this study. In addition, technologies that capture the most CO_2 per unit energy, such as BECCS in power or hydrogen production, become less competitive when CO_2 sequestration resources are limited, which reinforces the preference for allocating biomass to liquid fuels in our results. These system-level insights are mostly insensitive to changes in assumptions regarding fossil and alternative fuel supply flexibility, their costs, as well as to the assumed fuel demand distribution. This is illustrated in Fig. 10, which highlights the share of biofuels, fossil fuels, and synthetic fuels across all evaluated cases under different biomass availability and CO_2 sequestration assumptions.

Across the evaluated net-zero energy systems, low-carbon fuels play a major role in meeting liquid fuel demand, but their contribution to gaseous fuel supply remains limited, except when the cost of producing alternative liquids is substantially increased and resources are more constrained. This result reflects the lower abatement cost of alternative liquid fuel pathways relative to gaseous fuel pathways, driven by the lower carbon intensity and cost of fossil natural gas compared to fossil liquids assumed in this study.

The modeling results also reveal large variations in system-wide hydrogen consumption, with the most demand – nearly eight times the demand in the case with the least hydrogen consumption – occurring in scenarios with the greatest synthetic fuel production. As hydrogen use increases under limited CO_2 sequestration, this additional demand is satisfied using electrolytic hydrogen production, which increases overall electricity demand and low-carbon power generation. In this way, constraints on biomass availability and CO_2 sequestration are managed through an expansion of low-carbon electricity supply, largely VRE generation, which itself may be limited by policy or societal constraints not considered in this analysis.[41,59]

All net-zero scenarios exhibit substantial increases in biomass primary energy, CO_2 sequestration, electricity generation, and in some cases, hydrogen production. CO_2 sequestration and hydrogen increase the most relative to today, although hydrogen production varies considerably by scenario. On the other hand, among the different types of energy that expand, electricity increases the most in absolute terms.

Finally, the range of energy system outcomes resulting from varying constraints highlights tradeoffs that will need to be examined and managed as part of an energy transition. For example, scenarios differ in terms of system costs (scenarios with more stringent resource constraints are more costly) but also in terms of the amount and type of land use (*e.g.*, scenarios

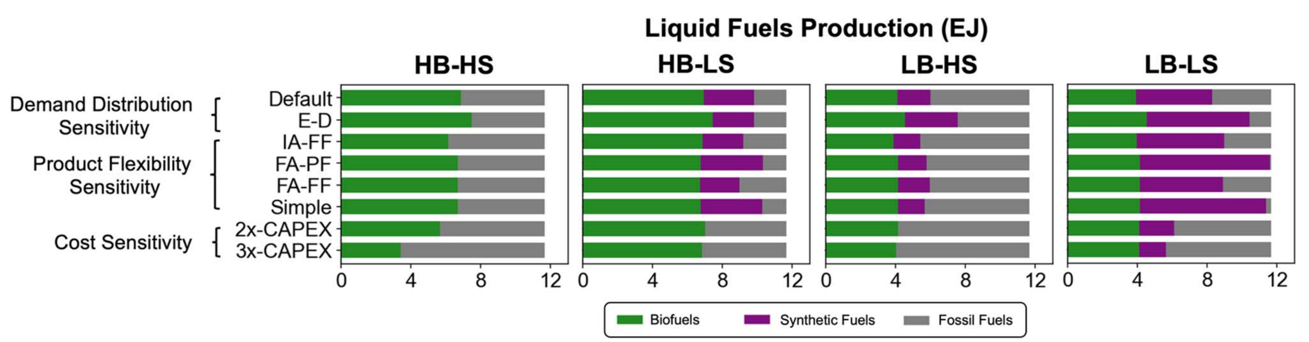

Fig. 10 Summary of liquid fuels production pathways (biofuels, synthetic fuels and fossil) across all core scenarios and sensitivity cases in the main text. "Demand Distribution Sensitivity" includes default and "E-D" demand distributions described in Fig. 2A under "IA-PF" modeling assumptions described in Fig. 3B. "Product Flexibility Sensitivity" includes "IA-FF", "FA-PF", "FA-FF", and "Simple" modeling assumptions described in Fig. 3B under default demand distributions. "Cost sensitivity" includes "2×-CAPEX" and "3×-CAPEX" that refer to doubled or tripled capital costs for bio and synthetic liquid fuels production technologies under default demand distributions and "IA-PF" modeling assumptions.

that use less land for bioenergy may require more land for electricity infrastructure). In addition, scenarios with limited bioenergy tend to use more CO_2 sequestration, illustrating that constraining one resource may put more pressure on another.[41]

From a policy perspective, these results highlight the importance of early development of CO_2 transport and storage infrastructure and clear governance of biomass resource allocation. Expanding CO_2 storage capacity reduces reliance on more energy-intensive synthetic fuel pathways and lowers overall system costs. Conversely, delays in developing CO_2 storage would shift the system toward greater deployment of hydrogen and electricity-intensive synthetic fuels, increasing the need for large-scale expansion of low-carbon power and hydrogen infrastructure.

4.2. Comparison with prior system-level studies on fuel decarbonization

A systematic comparison of our model results to those from other energy system studies on liquid fuel decarbonization is challenging, given differences in model structure (*e.g.*, temporal resolution of grid operations, sectoral scope and interactions), technology parameterization, and demand assumptions. Nevertheless, documenting similarities and differences remains valuable, as it highlights the sensitivity, or insensitivity of certain outcomes to modeling and data assumptions and underscores the need for further analysis to resolve discrepancies across models and scenarios. In this context, our finding that synthetic fuel deployment is driven primarily by constraints on CO_2 sequestration (and less so on biomass availability) agrees with the findings of several other studies focused on fuel decarbonization pathways that consider sector-coupled energy systems frameworks.[35,41,60,61]

The continued role of fossil liquids and their sensitivity to available CO_2 sequestration is consistent with findings from other studies that explicitly examine competition among biofuels, synthetic fuels, and fossil fuels.[3,35,41,62] Fewer studies, however, examine how product distribution constraints affect the competitiveness of fossil liquids. We find that these constraints only modestly affect the relative competition between fossil fuels, biofuels, and synthetic fuels (Fig. 8), but they play a larger role in altering the competition among alternative fuel production technologies.

Even though there is broad agreement among energy system modeling studies about the importance of biomass as a means to provide atmospheric carbon for CDR to achieve deep decarbonization, there is less consensus on technological pathways for biomass utilization across electricity, H_2, gaseous fuel, and liquid fuel production sectors.[3,35,41,62–65] As pointed out by other studies,[62] it is difficult to glean insights about the disposition of biomass when opportunities to deploy BECCS in different sectors are not consistently represented in models. For instance, in contrast to our finding that biomass is used entirely for biofuel production, Millinger *et al.*, who examine the role of biomass in a high-electrification European decarbonization context using a multi-sector CEM framework,[35] report a relatively small role for biofuels, with biomass primarily allocated to heat and power generation. However, biomass will tend to be utilized in sectors in which it can be coupled to CCS, so this result may reflect the lack of assumed availability of CCS on biofuels production in that study than anything more fundamental.

The existence of several near-optimal solutions in CEMs with several binding constraints, which is common under deep decarbonization scenarios,[66] also creates the possibility that small deviations in assumptions could lead to differences in biomass utilization. This point is evident in our cost sensitivity analysis (Fig. 9), in which BECCS shifts from liquid fuels to H_2 production under high capital cost assumptions for liquids, but only when biomass and CO_2 sequestration resources are abundant. This sensitivity illustrates that the sectoral allocation of biomass depends not only on resource availabilities, but also on technology cost assumptions of both biofuels and competing uses of biomass.

4.3. Insights regarding fuel production technologies and their representation in system models

Our analysis highlights several key takeaways for alternative fuel technology development and associated process-level assessment. First, the optimal liquid fuel decarbonization pathways across the evaluated biomass and CO_2 sequestration assumptions rely on high CC rates (>70%) associated with biofuel production. This suggests a need for closer process-level examination of the incremental energy and non-energy cost requirements (*e.g.*, capital costs) associated with increasing CC rates in biofuel processes.

Second, the system-level integration of biofuel and synthetic fuel production increases the fraction of atmospheric carbon converted to fuel under resource-constrained scenarios. This increase in carbon conversion efficiency highlights the potential value of novel processing strategies that enhance biofuel carbon conversion. Specifically, rather than using CO_2 as a feed, using biomass as a feed while making process changes to recover and convert process carbon as part of the same biofuel production process could improve overall efficiency.[67,68] Such approaches would have the added advantage of increasing biomass conversion efficiency, which could be valuable if biomass feedstocks are limited or costly and could help to diminish concerns about the land use implications of bioenergy production. On the other hand, increasing the conversion efficiency of biogenic carbon would increase the demand for hydrogen and electricity for fuels production.

Third, the sensitivity of fuel process selection to assumptions about product demand distribution underscores the need to characterize the incremental costs and energy requirements associated with varying product slates at the process level. There is a similar need to understand the flexibility of incumbent refineries and the incremental costs associated with changing product slates. In general, consistency in assumptions across different fuel production processes with different capture rates, product slates, and feeds would be very useful for evaluating the competitiveness of these technologies in scenarios generated by system models.

Finally, unlike sectors such as electricity and H_2, in which technology alternatives are well-characterized and can often be represented in energy system models with relatively few parameters, analyzing liquid fuel decarbonization pathways requires extensive data integration between process-level engineering (including TEA) models and energy system models. In this context, greater transparency and rigor in documenting process-level studies – including the ability to track carbon and energy flows within the process – would facilitate consistent parametrization of competing fuel technologies in energy system models, even when sourced from multiple, heterogeneous process-level studies. For example, reporting the cost factors used to scale equipment costs to total overnight costs could help harmonize these scaling factors across similar technologies before they are applied in energy system models.

4.4. Study limitations and future directions

We identify several study limitations that point towards areas for future work. First, we did not consider the time path of fuel technology deployment between the present and the net-zero year (nominally 2050), thereby omitting possible path dependencies driven by near-term policy or market dynamics. Instead, the single-year formulation represents a future system configuration that satisfies net-zero emissions under specified demand, technology, and resource conditions and is used to identify the system-level drivers of fuel pathway competition under deep decarbonization. As the results are primarily governed by long-run resource constraints such as biomass availability and CO_2 sequestration capacity, transition dynamics such as technology learning, deployment rates, or policy timing are unlikely to fundamentally alter the relative roles of liquid fuels pathways identified here, although they may affect the timing, and associated costs of technology deployment.

Near-term investment decisions may also create path dependencies that affect long-run outcomes. The rate of development of low-carbon infrastructure, such as carbon capture retrofits, CO_2 transport and storage networks, and low-carbon hydrogen systems, could alter the decarbonization trajectory and associated transition costs. For example, if carbon capture retrofits are applied to existing corn ethanol facilities, which were excluded in our analysis, it is possible that these would deploy and would continue to be economic under deep decarbonization. However, this would primarily influence the utilization and timing of existing assets rather than the long-run fuel mix, which is predominantly determined by system-wide biomass availability and CO_2 sequestration constraints. Second, although our analysis incorporates supply curves for various renewable energy and carbon storage resources, we adopt simplified assumptions for fossil liquids and natural gas. This reflects the expectation that fossil fuel utilization will decline under deep decarbonization, reducing the likelihood that supply constraints will materially affect outcomes.

In addition, while our analysis included multiple technological pathways for biofuels, we represented only a single Fischer–Tropsch pathway for synthetic liquid fuels with a fixed product distribution, reflecting the focus on jet-dominant processes in the literature. This representation limits our ability to evaluate liquid fuel demand distributions that diverge substantially from current patterns, particularly under constrained biomass and CO_2 sequestration availability. Alternative synthetic fuel pathways may differ in terms of carbon conversion efficiency, which would affect the associated hydrogen and electricity demand. We approximated this effect within a single pathway by considering variants with different extents of CO_2 capture and recycling (Table S33). Our results suggest that higher carbon utilization pathways are generally preferred when CO_2 sequestration is constrained and *vice versa*. Sensitivity analyses on fuel demand distribution (Section 3.4) and product flexibility (Section 3.5) further indicate that changes in product slates have a limited impact on the aggregate roles of biofuels, synthetic fuels, and fossil fuels, as well as on the technology mix in other sectors, although they do affect the contributions of individual fuel technologies. Consequently, expanding the representation of synthetic liquid fuels options to include a broader range of capital costs, operating costs, and energy intensities, in addition to alternative product slates, is therefore an important priority for future work.

We also note that an increasing share of synthetic fuels leads to higher average liquid fuel prices,[35] which could incentivize reductions in liquid fuel demand in favor of direct electricity use or deployment of other energy carriers such as H_2. Although not explicitly modeled here, such final energy demand substitution would likely result in lower total electricity and H_2 generation due to the increased energy efficiency of direct electrification *versus* its indirect use to produce synthetic fuels. Therefore, improving the characterization of fuel demand elasticity to fuel prices in energy system models could further clarify the role for synthetic fuels in energy system decarbonization pathways.

Similarly, more information about variation in future final energy demands for both liquid fuels and other energy commodities would enable exploration of a wider scenario space. Lower aggregate fuel demand under the same biomass and CO_2 resource assumptions could reduce the sensitivity of fuel technology deployment to resource constraints, while higher demand driven by growth in fuel-intensive services (*e.g.*, aviation) or a slower rate of electrification could amplify the importance of these resource constraints. In addition, there are substantial opportunities to more explicitly integrate fuel production with carbon-intensive industrial sectors (*e.g.*, chemicals production) to capture competition for feeds as well as co-production of fuels and chemicals that could alter process selection across sectors.

While the MACRO framework can represent diverse biomass resources and plant configurations, the present case study does not explicitly model facility siting, intra-regional transport distances, or detailed supply chain logistics. Such features would require substantially finer spatial resolution and are beyond the scope of this system-level analysis. In addition, this study did not consider other greenhouse gases or indirect climate effects, which are typically smaller in aggregate and more uncertain than greenhouse gas effects.[69]

5. Conclusion

This study examines liquid fuel decarbonization pathways using a multi-sector capacity expansion modeling framework applied to a net-zero case study of the contiguous United States. We find that two factors – biomass and CO_2 sequestration resource constraints – shape competition among biofuels, synthetic fuels, and fossil liquids, as well as the overall disposition of atmospheric carbon in the energy system. Biomass availability determines the extent of biofuel deployment and CO_2 capture rates in liquid fuel production pathways, whereas CO_2 sequestration availability governs the balance between carbon storage and utilization for synthetic fuels production.

These system-level findings are robust to assumptions regarding liquid fuel demand distributions, production flexibility, and variations in capital cost. At the same time, these assumptions shape competition among biofuel processes, as process selection is the primary means by which fuel supply is aligned with the product demand distribution. Moreover, the utilization of captured biogenic CO_2 for synthetic fuel production under resource-constrained scenarios enhances the overall conversion of atmospheric carbon to liquid fuels, highlighting the potential value of coordinated process development and system-level integration.

Finally, the implications of this analysis extend beyond the liquid fuels sector. Increased reliance on synthetic fuels would inherently link liquid fuel decarbonization to large-scale deployment of low-carbon hydrogen and electricity, highlighting the potential value of coordinated cross-sector infrastructure planning. In addition, future research could examine the temporal evolution of these pathways, broaden the representation of synthetic fuel technologies with diverse product distributions, incorporate endogenous fuel demand responses, consider other assumptions about final energy demands, and improve the representation of industrial sector coupling. Collectively, these extensions would enable a more comprehensive understanding of alternative transition pathways toward net-zero energy systems.

Author contributions

J. W. L: methodology, software, formal analysis, investigation, data curation, writing – original draft, visualization. B. K. M: conceptualization, formal analysis, writing – review and editing. D. S. M.: conceptualization, formal analysis, supervision, writing – review and editing.

Conflicts of interest

There are no conflicts of interest to declare.

Data availability

All data supporting this article are provided in the supporting information (SI). Supplementary information: additional results for the core and sensitivity scenarios; description of methods; modeling input assumptions; carbon balances of alternative fuels technologies; model implementation detailsds descrdocumentations of fuels modeling in the MACRO model. See DOI: https://doi.org/10.1039/d5se01654a.

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