nature portfolio

Peer Review File

Diverse Decarbonization Pathways Under Near Cost-Optimal Futures

REVIEWER COMMENTS

Reviewer #1 (Remarks to the Author):

The paper analyses 240 near-cost-optimal energy system decarbonisation pathways generated via 'Modelling to Generate Alternatives' (MGA). The aim is to identify technologies that are consistently deployed across such pathways, which may represent 'no-regret' investment options, as opposed to technologies whose role is more volatile across pathways. The study relies on the well-established open-source energy system modelling framework Temoa and focuses on the US energy system.

The study is original for two reasons. First, as the authors state, it is the first study performing such kind of analysis for the US energy system. Second, it is one of the few studies applying MGA to energy system decarbonisation pathways, including all energy sectors. In fact, most recent MGA studies applied to energy systems relied on models that do not take into account capacity deployment through time but only the end state of the designed system. This second element of novelty (and the computational challenges it entailed, as mentioned in the Supplement) could be better emphasised.

Nonetheless, some aspects of the study require further clarification or expansion before it can be published in this Journal.

The first aspect pertains to the methods. The whole analysis is based on the generated set of 240 near-optimal solutions, which the authors obtain via a version of MGA based on randomised weights, similar to previous work in the literature but still unique in the way weights are applied to 'activity' variables instead of capacity ones.

The method, however, would require further clarification: it is not explicit how exactly this weighting of activity (which I interpret as flows in and out) variables works in the context of pathways. How often are activities accounted for along TEMOA's multi-decadal pathways? Is the weighing occurring only for the total activity over multiple years or separately for each dispatch horizon (assuming there is more than one)? I assume the first, or you would have different sets of options branching out exponentially for each dispatch horizon, but (if correctly interpreted) this needs to be made explicit.

Furthermore, the authors do not provide any evidence supporting the legitimacy of the choice of this specific MGA method in relation to the type of statistical analysis they carry out for the obtained option space. For instance, how well does this particular version of MGA map the feasible option space for your particular model? Are 240 options a statistically meaningful sample to draw the type of conclusions you draw or not? Is there any risk that relevant options may have been omitted by the particular MGA search adopted? A few recent studies in the literature showed that MGA approaches like the one employed in this study are most likely not capturing all the feasible design options for a large energy system model and finite computational power. Instead, they will capture a subset of those, which can differ substantially depending on the chosen search strategy (i.e., which variables are weighted and how, what strategies, if any, are put in place to capture the extremes of the option space, etc.). In other words, a deeper critical or quantitative analysis of the adopted MGA method is needed in relation to the type of 'statistical' claims that the study makes to check whether the method and the analysis are compatible.

A second aspect that I advise expanding pertains to the results. Assuming that the concerns above the chosen MGA method are addressed, and the legitimacy of the method is corroborated, some of the obtained results are still unsurprising. For instance, the fact that renewables and storage tend to play a key role is rather well-established: is anybody suggesting that the energy transition could be better, or even possible, without large amounts of renewables and storage? Similarly, the fact that coal power without CCS is not an option across all pathways is something well-established, which most studies do not even bother investigating, given that a coal phase-out is what most countries are prioritising or have already achieved in their energy transition agenda. Finally, you show that many technological options for which there are viable alternatives are not must-haves, which is also unsurprising. With a modelling effort like the one put in place, you could look for more interesting multi-dimensional insights. For instance, while it is clearly possible to get rid of a given technology, say hydrogen, is it possible to do that while also getting rid of some other critical technology? In other words, what option space is left when avoiding one or more of those technologies on which we have less certain plans? Which technologies reduce the space remaining for other decisions the most and can be, therefore, considered more worthy of attention in the future? A deeper understanding of what kind of option space your MGA method offers, as suggested earlier, is critical to expanding the analysis in this direction.

In addition, there is little transparency concerning the model assumptions the analysis relies on. In particular, it is important to communicate if any assumptions might be driving the results in certain directions, especially regarding temporal dynamics. For instance, your option space shows that electrolysis becomes profitable only in later years, whilst blue hydrogen is attractive early on. Is this possibly driven by cost projections more than by other factors? This is just one example, but many similar cases could be made which call for a more transparent communication and critical discussion of the assumptions and their relation to the findings. In relation to this, it would be extremely important to carry out a sensitivity analysis for the most critical uncertain parameters in the model. In fact, while I agree that MGA mitigates to an extent the impact of parametric uncertainty, as the authors state in the introduction, it does not eliminate it entirely - the case of cost projections above being one example that MGA would not easily eliminate, except for very large accepted cost relaxations. Since you use a very narrow cost relaxation, I would advise performing a sensitivity analysis, at least on the main cost assumptions. This should be complementary to (and not a substitute for) a broader discussion of the main model assumptions.

Reviewer #2 (Remarks to the Author):

This study employs energy system modeling to explore a range of near cost-optimal net-zero CO2 pathways. While the topic of decarbonization pathways is significant, the study faces methodological and research design challenges:

• Despite utilizing robust analysis methods, the study fails to contribute novel insights to the existing body of literature. The focus of the study is predominantly on technological and technical modeling, neglecting crucial economic, behavioral, and policy dimensions. Consequently, I suggest that the article is more suited for publication in 'Applied Energy' rather than 'Nature Communication'. The scope and analysis lack the diversity and interdisciplinary breadth required for the latter journal.

• Key terminologies, such as 'least-cost net-zero pathways' and 'cost-optimal decarbonization', lack precise definitions, leading to ambiguity. The paper would benefit from clearly defined research questions and hypotheses to enhance understanding and focus.

• Furthermore, the rationale for employing energy system optimization models needs strengthening. This should include a detailed explanation of the methods used to analyze path dependencies and near-cost implications.

• Section 2.5 necessitates further development to more effectively explain how carbon emissions are measured. Addressing the complexity of quantifying emissions within interconnected energy systems is crucial, especially concerning the electrification of building appliances, vehicles, and the adoption of solar energy. While the discussion on trade-offs is intriguing, it requires deeper exploration and detail.

• Overall, the study should emphasize the uniqueness of its research findings beyond technical modeling. The policy recommendations need to be more closely aligned and integrated with these findings for a cohesive and impactful conclusion.

Reviewer #3 (Remarks to the Author):

This study employs a modelling to generate alternatives (MGA) approach to address the issue of deviations from reality caused by deterministic methods not accounting for uncertainty.

1. Please compare the differences in outcomes, such as the probabilistic profile, between the MGA method and other methods like Monte Carlo analysis, stochastic programming, and robust optimization in addressing parametric uncertainty. Evaluate whether the results from the MGA method are more reliable and its advantages.

2. The paper models different sectors such as electric, buildings, industrial, and transportation sectors using different sources of profiles/inputs settings. The selection of these settings currently lacks consideration of the intersections between sectors and how they interact with each other. Moreover, it should further elaborate on how uncertainties like climate change impact load uncertainty, as well as the uncertainties in the performance of energy sources and end-use devices over long time scales.

3. In the analysis of near cost-optimal decarbonization pathways, how are technologies selected for application, and what is their contribution to decarbonization? For instance, the reasons for considering battery storage technologies but not thermal storage.

4. Please provide examples of how diverse near cost-optimal scenarios guide energy planning compared to deterministic modeling, and the penetration rates of technologies selected in these scenarios. This is to demonstrate the significance and originality of the research topic.

<u>Response to reviewer comments:</u>

NCOMMS-23-58018: Diverse Decarbonization Pathways Under Near Cost-Optimal Futures

To Whom It May Concern:

We would like to thank the editor and reviewers for their thoughtful and thorough review, and constructive remarks. We have modified the manuscript based on these comments to improve and clarify the text. Please find below detailed responses in **blue** text (with direct quotes from the revised manuscript shown in **bold**, "quoted" and *italic* and text) to the comments and suggestions offered by the reviewers (shown in normal text). All line numbers in our responses correspond to the tracked-changes version of the revised manuscript.

Best regards,

The Authors

Reviewer #1 (Remarks to the Author):

The paper analyses 240 near-cost-optimal energy system decarbonisation pathways generated via 'Modelling to Generate Alternatives' (MGA). The aim is to identify technologies that are consistently deployed across such pathways, which may represent 'no-regret' investment options, as opposed to technologies whose role is more volatile across pathways. The study relies on the well-established open-source energy system modelling framework Temoa and focuses on the US energy system.

The study is original for two reasons. First, as the authors state, it is the first study performing such kind of analysis for the US energy system. Second, it is one of the few studies applying MGA to energy system decarbonisation pathways, including all energy sectors. In fact, most recent MGA studies applied to energy systems relied on models that do not take into account capacity deployment through time but only the end state of the designed system. This second element of novelty (and the computational challenges it entailed, as mentioned in the Supplement) could be better emphasised.

We thank the reviewer for recognizing the novelty of our work. We believe that these aspects – namely the expansive nature of conducting this study on the full U.S. energy system and the ability to consider capacity expansion over time – are key contributions. In our response to reviewer comments below, we demonstrate how we better communicate these important aspects of our study.

Nonetheless, some aspects of the study require further clarification or expansion before it can be published in this Journal.

1. The first aspect pertains to the methods. The whole analysis is based on the generated set of 240 near-optimal solutions, which the authors obtain via a version of MGA based on randomised weights, similar to previous work in the literature but still unique in the way weights are applied to 'activity' variables instead of capacity ones. The method, however, would require further clarification: it is not explicit how exactly this weighting of activity (which I interpret as flows in and out) variables works in the context of pathways. How often are activities accounted for along TEMOA's multi-decadal pathways? Is the weighting occurring only for the total activity over multiple years or separately for each dispatch horizon (assuming there is more than one)? I assume the first, or you would have different sets of options branching out exponentially for each dispatch horizon, but (if correctly interpreted) this needs to be made explicit.

We thank the reviewer for highlighting this. The reviewer's understanding of the application of the objective function is correct. The objective function serves as a "search" function in the near-cost optimal decision space as in other studies that employ MGA. In the present study we chose activity variables as the basis of this search as we were interested in exploring diversity in the solution space with respect to the actual contribution of each technology in the model towards meeting intermediate or end-use demands in the model. Other works have used capacity variables in the past as noted by the reviewer.

We provide the following clarifications to our methods:

- **The activity of the decision variables is indeed the flow or use of that technology within the model. It is this parameter that is weighted using a scalar from the uniform distribution.**
- **Activities for each technology are accounted for at each time step (as well as for each region in the model)**
- **When applying the weighting, the activities are summed together to represent a total activity over the multiple years, and it is this value that is assigned a weight in the MGA search algorithm.**

The following changes have been made to the revised manuscript to make the application of our MGA objective function mode explicitly as per the suggestions of the reviewer (Line 735 - 749):

"The addition of this slack allows for exploring near-optimal solutions in the decision space by accepting a small increase in the total system cost relative to the optimal solution. Additionally, the objective function in MGA runs is reformulated to emphasize a search direction. In this work, the objective function minimizes the sum of weighted activity (or flow) of technologies across the time horizon in the model, i.e. each technology is represented by a cumulative activity across the model time horizon. The technology representation in the current work is diverse and all technologies are chosen agnostically to be a part of the objective function to influence the search direction. Weights were sampled from a uniform distribution [-1, 1], assigned independently for each activity, which allows for the development of larger solution diversity with fewer MGA runs. The activity variables are chosen instead of their capacity counterparts as they directly represent each technology's contribution towards meeting end-use demands."

2. Furthermore, the authors do not provide any evidence supporting the legitimacy of the choice of this specific MGA method in relation to the type of statistical analysis they carry out for the obtained option space. For instance, how well does this particular version of MGA map the feasible option space for your particular model? Are 240 options a statistically meaningful sample to draw the type of conclusions you draw or not? Is there any risk that relevant options may have been omitted by the particular MGA search adopted? A few recent studies in the literature showed that MGA approaches like the one employed in this study are most likely not capturing all the feasible design options for a large energy system model and finite computational power. Instead, they will capture a subset of those, which can differ substantially depending on the chosen search strategy (i.e., which variables are weighted and how, what strategies, if any, are put in place to capture the extremes of the option space, etc.). In other words, a deeper critical or quantitative analysis of the adopted MGA method is needed in relation to the type of 'statistical' claims that the study makes to check whether the method and the analysis are compatible.

The reviewer raises an important concern related to the method used to search the near-optimal decision space in this study. Often, the distinguishing factor between MGA studies is the structure of the objective function, which serves as a mechanism to search the near-optimal decision space. Here, we address how our methodological choices ensure a broad examination of the solution space and how our sample size is sufficiently large to ensure minimal gains from further expansion.

Specifically, in this study, we adopted a functional form that weights the activities (or flow) through all technologies in a model in random manner from a uniform distribution between -1 and 1. We were agnostic in our representation of which technologies are selected as part of the objective

function as we select all technologies in the model to be a part of the search. The technologies in the model are numerous: 1080 unique technologies, each assigned a random coefficient in an MGA iteration. The technologies in the model are also diverse, ranging from solar photovoltaic centralized power plants to top mount refrigerators to CNG trucks. This weighting approach captures technologies when they are essential. Even when a technology is down weighted, it does not disqualify its deployment, it is simply "disadvantaged".

A new section in the SI discussing MGA iteration termination criteria has been added in response to the reviewer's concerns (Section S4):

"Section S4: MGA iteration termination criteria

The near-optimal decision space in energy system linear problems is typically vast. For example, in our model, there are numerous (1080 unique technologies) and diverse technologies represented. A comprehensive search of this space can pose challenges due to its multi-dimensional nature. Recent methods in literature employ strategies that attempt to identify all feasible design options within the convex hull of the MGA solution space.[14] These methods use a subset of dimensions of interest, determined beforehand, in an algorithmic way with unit vectors to look for the decision boundaries of the near-optimal space. The current study employs a search function that weights the activities (or flow) through technologies in the model with a random weight sampled from a uniform distribution between -1 and 1. Activities are used in the objective function as they represent the contribution of each technology towards meeting intermediate or end-use demands. Allowing both positive and negative weights resulted in a more expansive set of solutions relative to "one-sided" weights (example: [0, 1]). Overall, this approach allows for an agnostic inclusion of all technologies in the model to influence the search direction in the convex hull, which is the primary tradeoff with other approaches where a small subset of technologies (or technology groups) are chosen as axes to search on apriori."

We also tested alternative weights that were "one-sided" (example: [0, 1]) and found that the range of solutions obtained was restricted compared to when we weighted with [-1, 1]. In this formulation, having both negative and positive weights allows for a more expansive examination of the near-optimal space relative to "one-sided" weights.

We have performed additional MGA runs and extended our analysis to cover >1,000 iterations to address the concerns regarding having a meaningfully large sample size of MGA iterations. In Figure S2 below, we provide the change in statistics as a function of MGA iteration for the quantities of interest covered in the main manuscript. There is little change in the distributions in almost all cases after 300-400 iterations. We have amended the manuscript to now present results from 1,100 iterations of MGA.

Additional text is provided in Section S4:

"To illustrate that the number of MGA iterations from which statistics are drawn is sufficient, we provide the change in statistics as a function of iterations for the quantities of interest covered in the manuscript. There is little change in the distributions in almost all cases after 300-400 iterations."

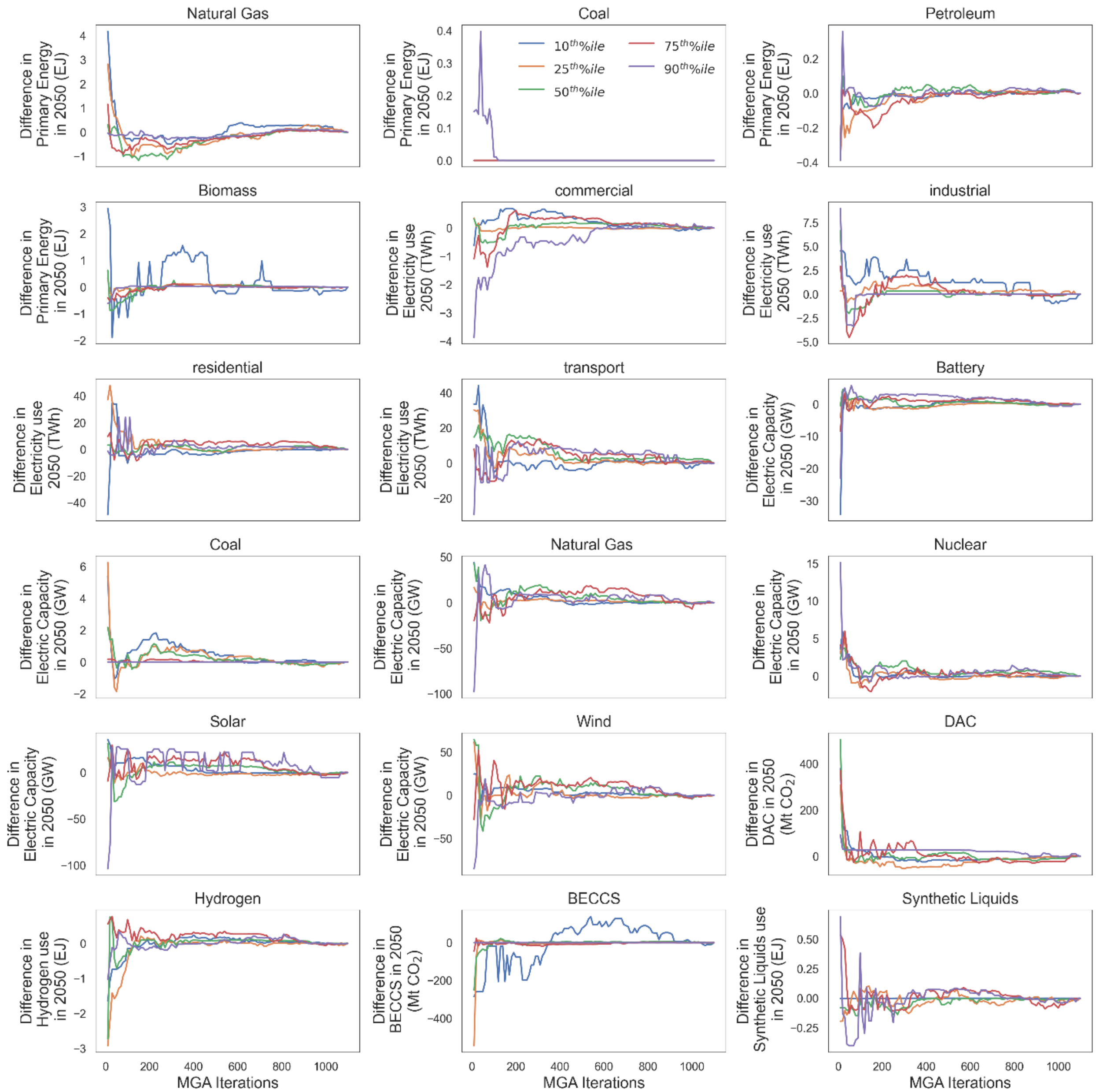

Figure S2: Convergence in statistics of parameters discussed in the manuscript as a function of MGA iteration (up to 1,100 iterations). The different colors in each panel show the 10th, 25th, 50th, 75th, and 90th percentile values for the different parameters. The plot presents the convergence of primary energy use of fossil fuels, electricity use by sector, electric capacity, and carbon mitigation technologies.

We do, however, acknowledge that in a multi-dimensional space such as the one in consideration here, even an extended number of iterations is liable to omit configurations of the energy system in the near-optimal space. It is possible that the structure of our search function (objective function) is unable to find certain configurations of the energy system, no matter the number of iterations of MGA we run. Other methods published in the literature attempt to capture all modeling

alternatives, using a subset of dimensions of interest in a more algorithmic way along with unit vectors to look for the decision boundaries of the near-optimal space. Such methods capture the extremes of the option space in a more structured manner than the method adopted in the current work. These approaches are not computationally feasible for a multi-decadal capacity expansion approach that considers thousands of activity variables. Faced with the tradeoff of limiting the analysis to a subset of energy system decisions or pursuing the broadest exploration of the solution space, we opted for the former, as we were interested in a search agnostic of any pre-held notions by analyzing results while using all technologies as part of the optimization in the spirit of addressing structural uncertainties in the model. We find that >95% of the activities are responsive to our MGA approach, with 75% of activities (from the 1080 unique technologies) exhibiting coefficients of variation larger than 20% as a response to the MGA approach deployed. This illustrates that our approach is capturing a wide range of possible futures within the solution space.

To better articulate the advantages and limitations of our approach, we update the text to acknowledge that the MGA formulation is not fully exhaustive in its exploration of the near-optimal decision space, while also demonstrating the extent to which the MGA formulation impacted a large number of decision variables. Based on the diminishing returns of increasing the number of MGA runs, we also assert that the distribution of results we present are comprehensive for the subset of the complete near-optimal decision space.

Additional text is provided in Section S4:

"However, in a multi-dimensional space such as the one in consideration here, even an extended number of iterations may not be sufficient to capture all energy system configurations of interest. It is possible that the structure of the search function (objective function) in the current study is unable to find certain configurations of the energy system. Adoption of this approach comes with a tradeoff of not having complete assurance of a comprehensive search in the near-optimal decision space. Applying the weighting factors directly to activity variables, however, ensures a broad response in the model. In our formulation of MGA, we see more than 95% of activities vary, with 75% of activities showing a coefficient of variation larger than 20% in response to different weighting factors, illustrating the breadth of the solution space that is being explored. This shows that our approach is capturing a wide range of possible futures within the solution space."

We have also ensured that the range of solutions presented in the manuscript is not implied to be a comprehensive set of possible futures; instead, they reflect the range of solutions derived from our adopted MGA method.

3. A second aspect that I advise expanding pertains to the results. Assuming that the concerns above the chosen MGA method are addressed, and the legitimacy of the method is corroborated, some of the obtained results are still unsurprising. For instance, the fact that renewables and storage tend to play a key role is rather well-established: is anybody suggesting that the energy transition could be better, or even possible, without large amounts of renewables and storage? Similarly, the fact that coal power without CCS is not an option across all pathways is something well-established, which most studies do not even bother investigating, given that a coal phase-out is what most countries are prioritising or have already achieved in their energy transition agenda. Finally, you show that many technological options for which

there are viable alternatives are not must-haves, which is also unsurprising. With a modelling effort like the one put in place, you could look for more interesting multi-dimensional insights. For instance, while it is clearly possible to get rid of a given technology, say hydrogen, is it possible to do that while also getting rid of some other critical technology? In other words, what option space is left when avoiding one or more of those technologies on which we have less certain plans? Which technologies reduce the space remaining for other decisions the most and can be, therefore, considered more worthy of attention in the future? A deeper understanding of what kind of option space your MGA method offers, as suggested earlier, is critical to expanding the analysis in this direction.

Thank you for this comment and for prompting a more detailed exploration of our findings. While it is appropriate that some of our results are consistent with the conventional wisdom, we expanded our results to explore more fully the extreme pathways. In particular, we sought to better understand technology choices in pathways when other technologies are either abundant or scarce. To do this, we have added a section in the SI in which we recreate our distributions for the MGA runs using only a subset of the results that include the top 10% or the bottom 10% of runs regarding the use of (1) hydrogen, (2) DAC, (3) synthetic fuels, and (4) BECCS. The associated text discusses some of the interesting findings:

Line 554 - 558 in the main text:

"In relation to fossil fuels, increased hydrogen use leads to reduced coal consumption but has a less dramatic impact on natural gas consumption (Section S6). While hydrogen commonly replaces natural gas in the industrial sector, this negative relationship is dampened due to pathways in which hydrogen is produced via steam methane reforming."

Line 563 - 567 in the main text:

"The positive correlation between biomass and synthetic liquids arises from the link between hydrogen and synthetic liquids (the latter uses the former for synthesis via the Fischer-Tropsch process). High synthetic fuel use narrows the range of outcomes in the power sector, most notably eliminating coal CCS plants (Section S6)."

Line 589 – 593 in the main text:

"However, when hydrogen facilitates the production of synthetic liquid fuels, DAC becomes necessary to capture resulting CO_2 emissions. Figure 6c also shows competition between biomass and DAC, which Section S6 shows is driven by BECCS."

Section S6 added to the supplementary information:

"Section S6: Technology Choices with Varied Availability of Nascent Technologies

This section explores technology/energy carrier choices when technologies that are still in nascent stages for large-scale use are either abundant or scarcely available. We analyzed subsets of the MGA runs, including the top 10% or the bottom 10% regarding the use of: 1) hydrogen, 2) DAC, 3) synthetic fuels, and 4) BECCS.

Low and high hydrogen: Figure S6 shows that scenarios with higher hydrogen use greatly reduce coal consumption relative to low hydrogen use scenarios through the modeling horizon. However, coal is eliminated across both scenarios by 2050. Low hydrogen scenarios also result in a narrowing of natural gas use outcomes. Scenarios with low hydrogen availability create a lower ceiling for BECCS. These scenarios are also associated with higher DAC use to accommodate the loss of a low/zero carbon energy carrier.

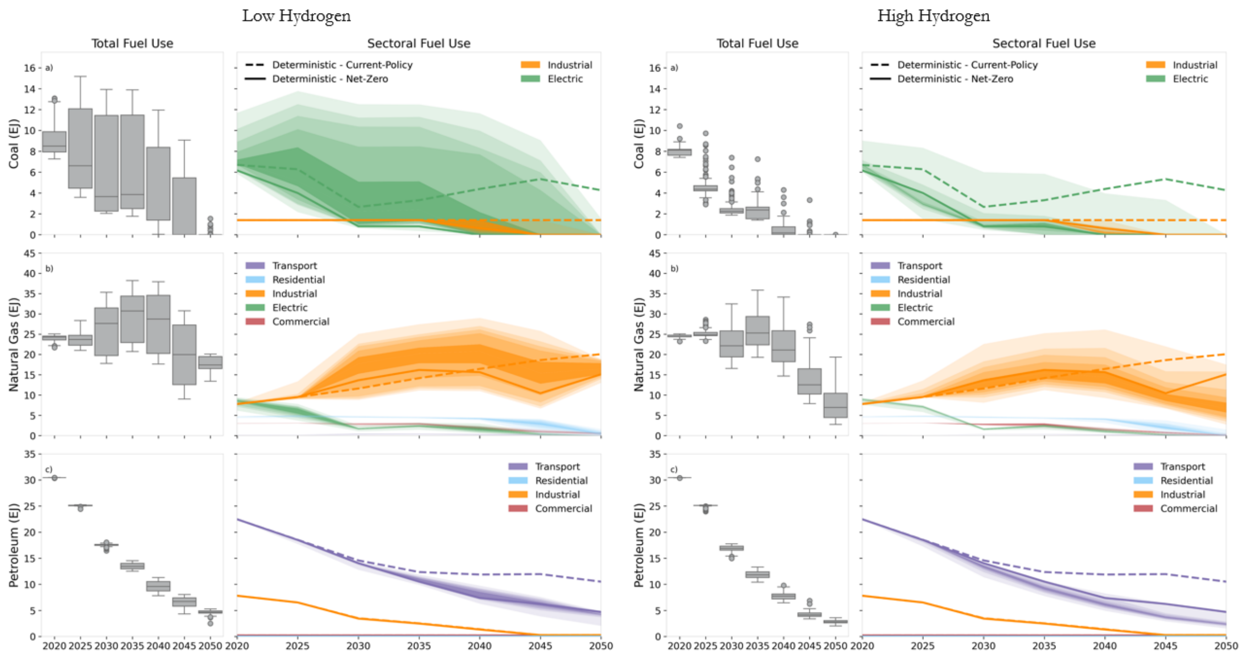

Figure S6: Near cost-optimal pathways for a) coal, b) natural gas, and c) petroleum in net-zero CO_2 pathways as presented in the manuscript. The left plot shows pathways with low hydrogen production as defined by the lowest 10th percentile of all 1100 MGA iterations (thus representing results from 110 MGA runs). The plot on the right represents the same but for the highest 10th percentile of hydrogen production pathways.

Low and high DAC: Figure S7 shows that scenarios with lower DAC use are associated with higher hydrogen use. These lower DAC scenarios were also associated with fewer instances of low BECCS. This relationship has also been observed in other work.[15] Unsurprisingly, scenarios with high DAC are associated with increased natural gas consumption compared to low DAC scenarios.

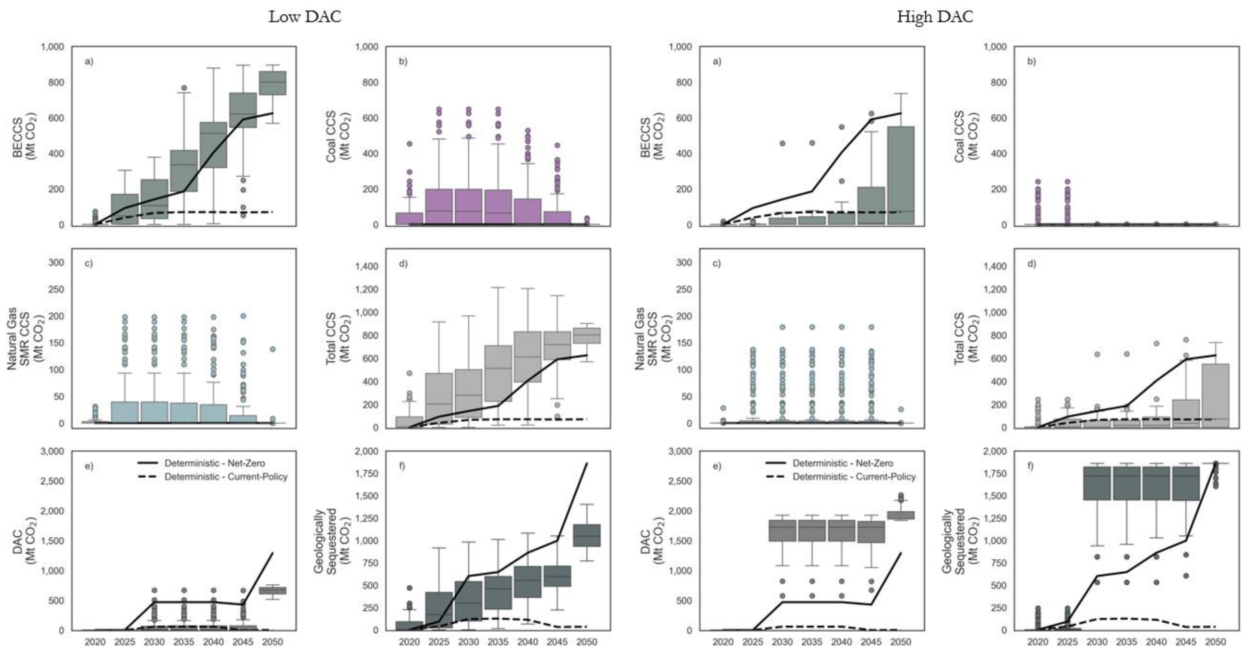

Figure S7: The box plots show the deployment of a) bioenergy with carbon capture and storage (BECCS), b) coal power with carbon capture and storage (coal CCS), c) natural gas steam methane reforming with carbon capture and storage (natural gas SMR CCS), d) total carbon capture and storage (CCS) as the sum of BECCS, coal CCS, and natural gas CCS, e) direct air capture (DAC), and f) total geologic sequestration as presented in the manuscript. The left plot shows pathways with low DAC use as defined by the lowest 10th percentile of all 1100 MGA iterations (thus representing results from 110 MGA runs). The plot on the right represents the same but for the highest 10th percentile of DAC use pathways.

Low and high synthetic fuel use: Figure S8 shows that scenarios with high synthetic fuel use result in the narrowing of outcomes from the power sector compared to low synthetic fuel use scenarios. High synthetic fuel use scenarios result in the elimination of coal CCS plants. While DAC levels by 2050 were comparable across the scenarios, the deployment of DAC starts earlier in the high synthetic fuel use scenarios. Unsurprisingly, hydrogen use in these high scenarios is also higher.

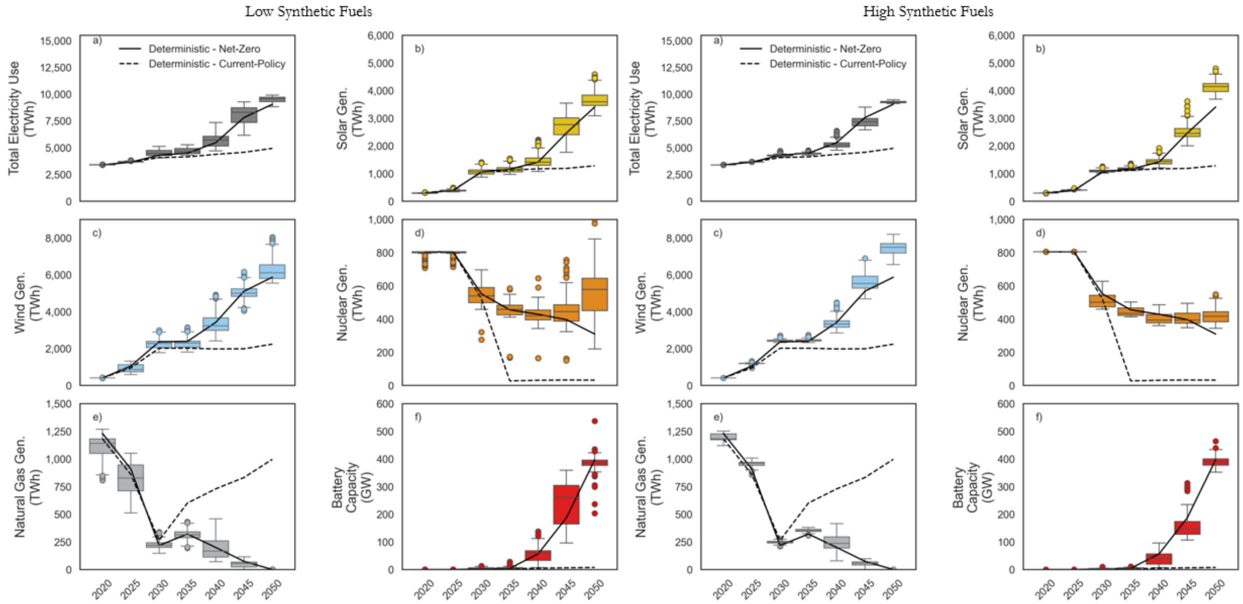

Figure S8: Near cost-optimal pathways in the power sector where box plots show a) total electricity use across the entire energy system, b) electricity generation from solar, c) electricity generation from wind, d) electricity generation from nuclear and e) electricity generation from natural gas all in TWh. Panel f) shows the battery capacity in GW deployed in the near cost-optimal decarbonization pathways as presented in the manuscript. The left plot shows pathways with low synthetic fuel use as defined by the lowest 10^{th} percentile of all 1100 MGA iterations (thus representing results from 110 MGA runs). The plot on the right represents the same but for the highest 10^{th} percentile of synthetic fuel use pathways.

Low and high BECCS: Figure S9 shows that scenarios with increased BECCS use see more coal consumption across the modeling horizon. As in the case of the high and low hydrogen use comparisons, coal is eliminated across both scenarios by 2050. Petroleum and natural gas largely show the same range of outcomes across the two scenarios.

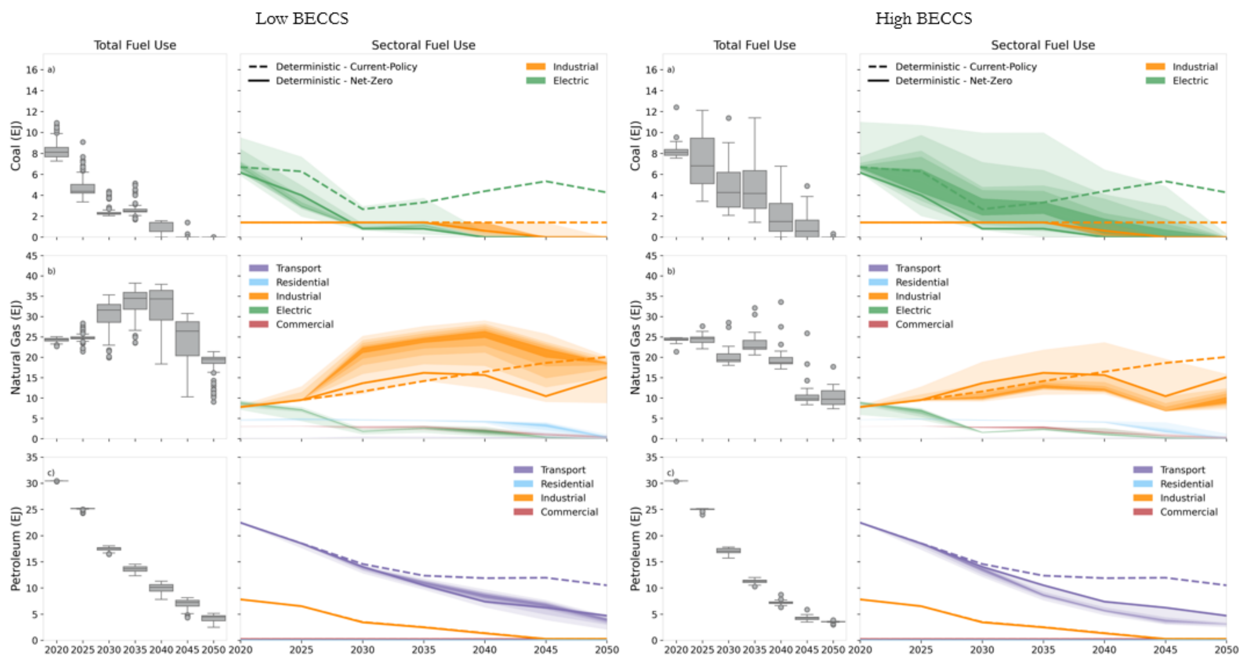

Figure S9: Near cost-optimal pathways for a) coal, b) natural gas, and c) petroleum in net-zero CO2 pathways as presented in the manuscript. The left plot shows pathways with low BECCS use as defined by the lowest 10th percentile of all 1100 MGA iterations (thus representing results from 110 MGA runs). The plot on the right represents the same but for the highest 10th percentile of BECCS use pathways.

4. In addition, there is little transparency concerning the model assumptions the analysis relies on. In particular, it is important to communicate if any assumptions might be driving the results in certain directions, especially regarding temporal dynamics. For instance, your option space shows that electrolysis becomes profitable only in later years, whilst blue hydrogen is attractive early on. Is this possibly driven by cost projections more than by other factors? This is just one example, but many similar cases could be made which call for a more transparent communication and critical discussion of the assumptions and their relation to the findings. In relation to this, it would be extremely important to carry out a sensitivity analysis for the most critical uncertain parameters in the model. In fact, while I agree that MGA mitigates to an extent the impact of parametric uncertainty, as the authors state in the introduction, it does not eliminate it entirely - the case of cost projections above being one example that MGA would not easily eliminate, except for very large accepted cost relaxations. Since you use a very narrow cost relaxation, I would advise performing a sensitivity analysis, at least on the main cost assumptions. This should be complementary to (and not a substitute for) a broader discussion of the main model assumptions.

As per the suggestions of the reviewer, we have conducted a limited parametric sensitivity analysis on some of the primary cost assumptions in the database, including fuel prices, the cost of renewables, and demand projections in a new SI section, Section S5: Sensitivity to input parameters. For energy system models of this size, advanced parametric sensitivity analysis methods, such as the Method of Morris, are the most appropriate for assessing the influence of all model parameters on model outputs. However, applying this method to our work is beyond the

scope of this analysis, especially since we are still in the process of developing the Method of Morris within the Temoa framework. This is also acknowledged in this new section in the SI.

"In this section we discuss the influence of uncertain inputs to the model: 1) the fuel prices, 2) cost of renewables and 3) demand projections in the residential, commercial, transportation and industrial sectors. The sensitivity of these input parameters is assessed against a subset of the major outputs from the model: 1) electric capacity, 2) electricity generation, 3) electricity use by sector, 4) energy system wide hydrogen production, 5) total primary energy use and, 6) the use of carbon management technologies in Figures S3-S5. For an ideal parametric uncertainty assessment of the model, advanced methods such as the Method of Morris should be employed. These methods are capable of comprehensively evaluating the influence of model parameters.

Sensitivity to renewable prices trajectories: Figure S3 shows the model results when the cost of renewables is perturbed from the "Moderate" market scenario as projected by the Annual Technology Baseline (ATB, Table 1). The ATB also publishes "Conservative" and "Advanced" market scenarios. Figure S3 demonstrates that, under a net-zero emissions constraint, these higher and lower cost perturbations result in minor changes in the deployment of electric capacity and generation resources over the modeling horizon. In the scenario with higher renewable costs, nuclear generation increases slightly, whereas it decreases in the scenario with lower renewables cost. Additionally, the higher renewables cost scenario results in reduced hydrogen production. Conversely, the lower renewables cost case results in an increase in hydrogen production.

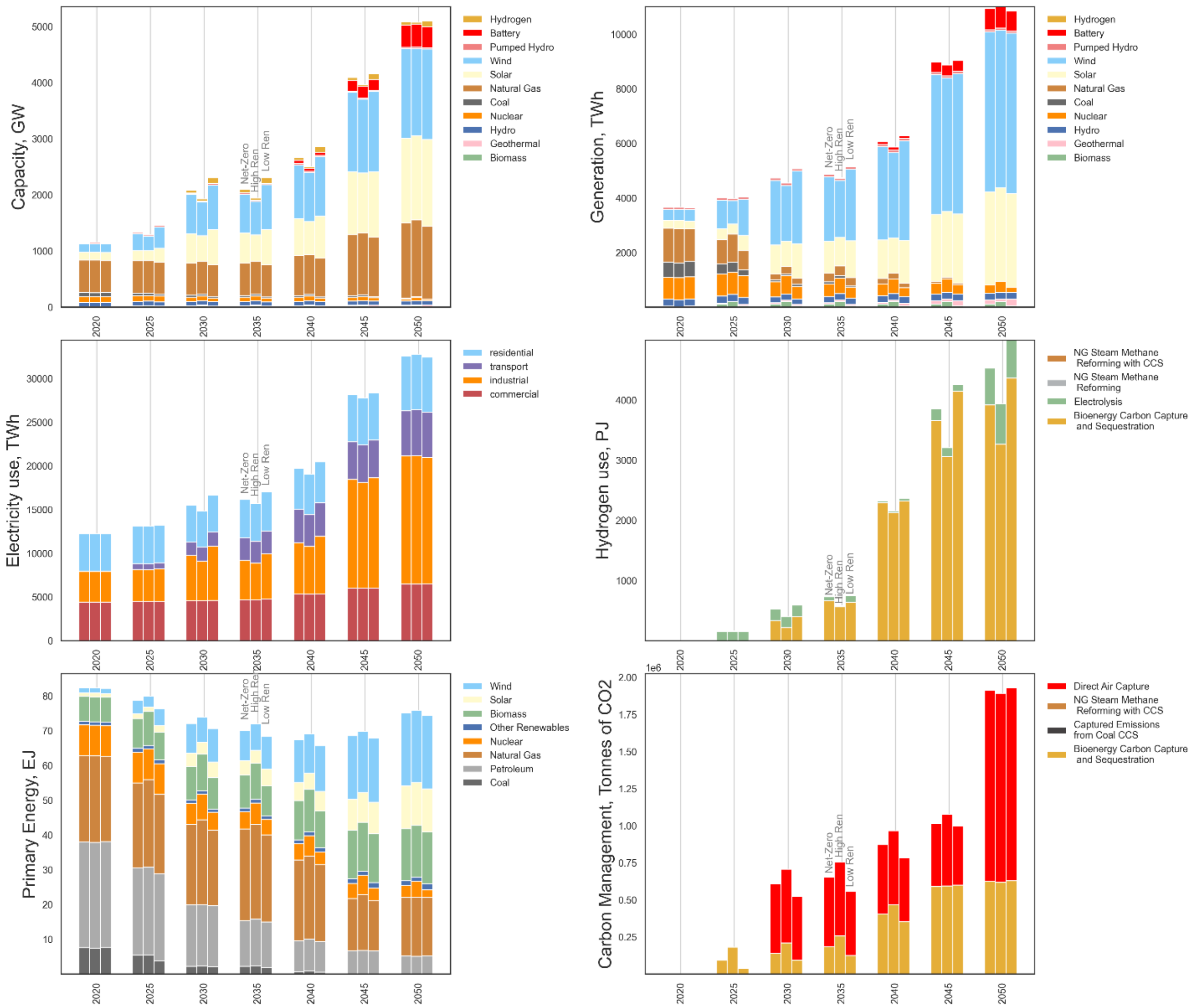

Figure S3: Sensitivity of renewable price trajectories as observed in: 1) electric capacity, 2) electric generation, 3) electricity use by sector, 4) hydrogen production pathways, 5) energy system wide primary energy use, and 5) carbon management technologies. The left bar represents the results with the moderate renewable cost assumptions (presented in the least-cost net-zero pathway in the manuscript), the middle bar represents a high renewables cost scenario, and the right bar represents a low renewables cost scenario.

Sensitivity to fossil fuel price trajectories: Figure S4 shows model results obtained by perturbing the fossil fuel prices from the "Reference" scenario projected by the Annual Energy Outlook (AEO, Table 1). The AEO also publishes "Low" and "High" fuel price scenarios. Figure S4 shows that these price profiles result in some notable changes across the modeling horizon. Electrification in the transportation sector is sensitive to petroleum prices, with a slower rate of electrification noted when petroleum prices are lower and a faster rate when prices are higher. By 2050, the total electricity use in the transportation sector is slightly higher in the scenario with higher petroleum prices compared to other scenarios. The high oil price scenario leads to substantial hydrogen production 2025 to 2050. In this scenario, the expensive transportation fuels are displaced by synthetic fuels created via the

Fischer-Tropsch process, using hydrogen in their synthesis. The primary energy panel in Figure S4 also highlights the difference in petroleum utilization across the sensitivity scenarios in response to the price profiles.

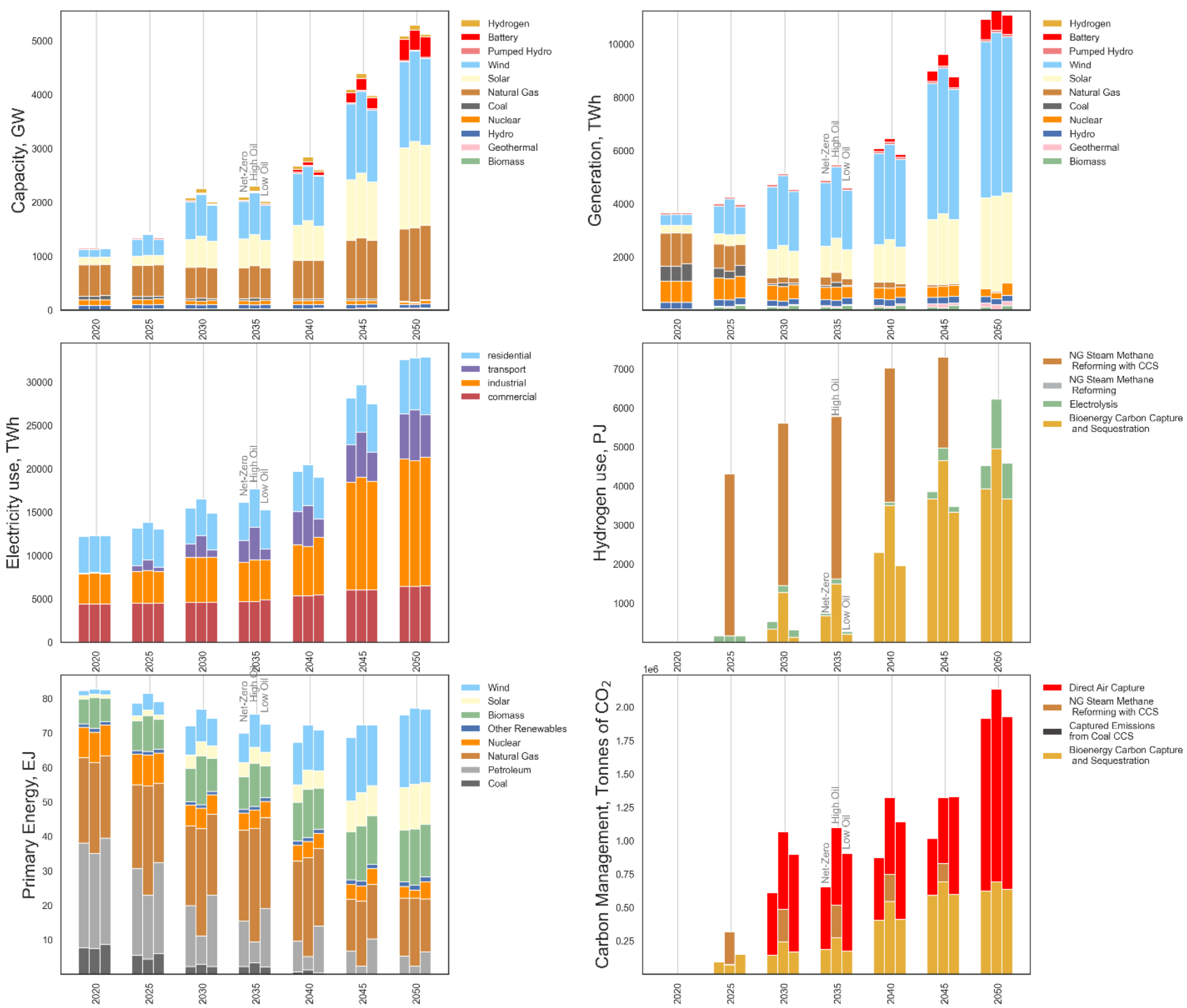

Figure S4: Sensitivity of fuel price trajectories as observed in: 1) electric capacity, 2) electric generation, 3) electricity use by sector, 4) hydrogen production pathways, 5) energy system wide primary energy use, and 5) carbon management technologies. The left bar represents the results presented in the least-cost net-zero pathway in the manuscript, the middle bar represents a high fuel price scenario, and the right bar represents a low fuel price scenario.

Sensitivity to exogenously specified demands: Figure S5 shows model results obtained by perturbing the exogenously specified demands for all service demands in the model by 10%. The service demands are sector-specific, and Section S7 provides details on the underlying assumptions for each of these demands. Figure S5 shows that nearly all of the displayed model outputs respond to perturbations in the demand across the modeling horizon. Notably, electricity demand is not exogenously specified but instead responds to changes in service demands from the buildings, transportation, and industrial *sectors. Lower service demands in these sectors translate to a reduced need for electricity, and vice versa. Hydrogen production follows this trend as well. In terms of primary energy, solar, wind and nuclear resources show the most variation across the scenarios. Finally, carbon management technologies are relatively stable by 2050, though they exhibit some variation earlier in the modeling horizon.*

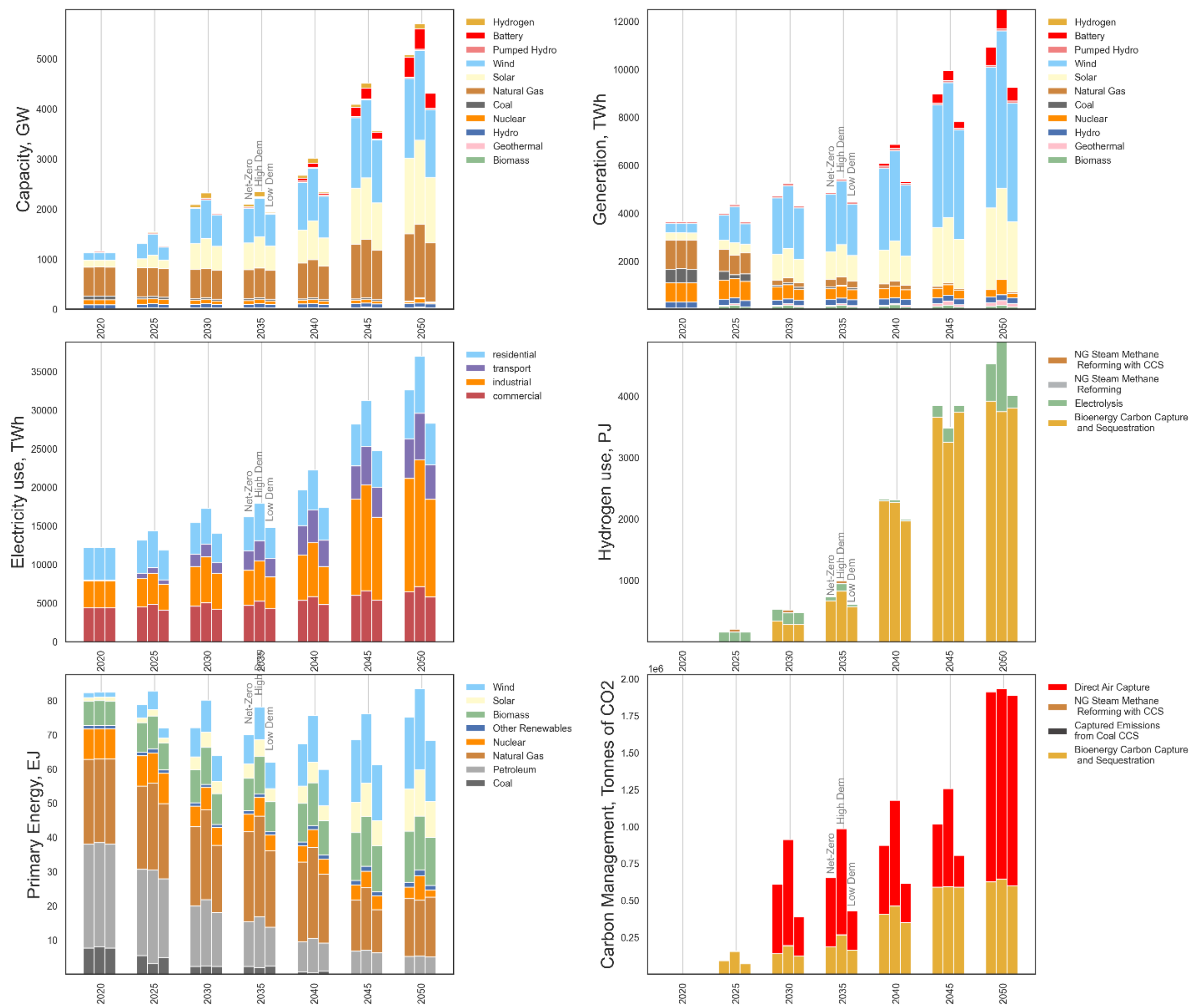

Figure S5: Sensitivity of exogenously specified demands as observed in: 1) electric capacity, 2) electric generation, 3) electricity use by sector, 4) hydrogen production pathways, 5) energy system wide primary energy use, and 5) carbon management technologies. The left bar represents the results presented in the least-cost net-zero pathway in the manuscript, the middle bar represents a high service demand scenario, and the right bar represents a low service demand scenario.

Uncertain input parameters have the potential to influence modeling results in a significant way. Here, we demonstrate that substantial variation in the model inputs results in model results that are fully encompassed in the range of results obtained from the MGA model runs. While this does not guarantee that all parametric tests or more stringent tests on the studied parameters will be inclusive of the MGA

results, it does demonstrate that the MGA approach is identifying near-cost-optimal results that include and extend beyond those from the standard parametric sensitivity analysis."

Reviewer #2 (Remarks to the Author):

This study employs energy system modeling to explore a range of near cost-optimal net-zero CO2 pathways. While the topic of decarbonization pathways is significant, the study faces methodological and research design challenges:

1. Despite utilizing robust analysis methods, the study fails to contribute novel insights to the existing body of literature. The focus of the study is predominantly on technological and technical modeling, neglecting crucial economic, behavioral, and policy dimensions. Consequently, I suggest that the article is more suited for publication in 'Applied Energy' rather than 'Nature Communication'. The scope and analysis lack the diversity and interdisciplinary breadth required for the latter journal.

We thank the reviewer for taking the time to review this work and also agree with the reviewer that dimensions, in addition to technological and technical modeling, would make for a strong submission to 'Nature Communication'. Economic and policy aspects are central to our work, and we are grateful to the reviewer for highlighting that these features were not sufficiently highlighted in the previous submission. In our opinion, the inclusion of these aspects allows this work to contribute meaningfully to the debate on the U.S. decarbonization landscape. The energy system model and accompanying database presented in this work are the result of insights from various interdisciplinary fields. As an energy system model, the sectors (buildings, transport, etc.) are all interconnected, and decisions made in one sector have the ability to influence those in other sectors within the model. Technology choice is endogenized in the model, and one of the primary considerations that the model uses in making these choices is the costs associated with these technologies. Section S7 discusses in some detail how each sector is represented and contains details on the underlying cost assumptions. For the deterministic run, the driving engine of the model is making economically cost-effective decisions where the goal is to obtain a least-cost solution to achieve net-zero targets. However, historical trends indicate that optimal decisions are seldom made when considering long-term energy system decisions. While we cannot reflect all aspects of behavior, this is part of the uncertainty we are trying to capture using the MGA method deployed. Finally, great care has been taken to represent U.S. policy appropriately in our model. For example, Section S8 details the provisions of the Inflation Reduction Act (IRA) and how they are parameterized in our model. Lines 659 - 667 have been added/amended in the manuscript to better highlight some of these points:

"Current and future U.S. policy will significantly shape the energy transition towards a net-zero CO_2 system. The debate over the optimal policy mechanisms to achieve this transition has been ongoing for decades. Existing policies have made progress towards decarbonization. However, our results suggest that reaching net-zero GHG emissions in the U.S. energy sector will require additional policy interventions after 2033, when key provisions of the IRA expire. Our results also highlight a large and diverse solution space for energy system decarbonization, in which technology deployment levels can vary widely. The results also indicate that deploying some technologies would lock in the need for synergistic technologies and push out the deployment of others."

The passage of the IRA in 2022 was a historical piece of legislation in the U.S. However, it is now clear that while the IRA has the potential to make a considerable decarbonization stride, it does not achieve net-zero conditions. Our results examine and highlight the gap between this historical piece of legislature and ambitious net-zero targets. The modeling effort shows us pathways to achieving this target, which could serve as useful policy directions for decision-makers. In a future where decarbonization is prioritized, this work could help inform policies for a "v2.0" of the IRA aimed at achieving decarbonization past this first iteration. The technical modeling in this work is particularly key as decisions in the real world are indeed influenced by economics. However, for a system as complicated as the energy system, this has been observed to not be the only factor in consideration. The modeling effort in the present work strikes a balance between optimal decision-making using a mathematical model while incorporating the "inefficiency" observed in the real-world.

2. Key terminologies, such as 'least-cost net-zero pathways' and 'cost-optimal decarbonization', lack precise definitions, leading to ambiguity. The paper would benefit from clearly defined research questions and hypotheses to enhance understanding and focus.

We thank the reviewer for pointing this out. The definitions for net-zero and least-cost pathways are now defined explicitly in the introduction. Least-cost and cost-optimal are used interchangeably, and this is also made clearer in the manuscript. We are open to other suggestions to improve the clarity/readability of the manuscript, but no other instances of unclear terminology were immediately obvious to us.

Line 46 - 48 of manuscript:

"In net-zero systems, the amount of CO2 emissions released into the atmosphere is balanced by the amount removed through various mechanisms such as carbon capture and storage, reforestation, or technological innovations."

Line 56 - 58 of manuscript:

"These models typically rely on least-cost optimization to inform decision-making, with investment and operational decisions achieving the lowest net present cost."

As per the suggestion of the reviewer, the research questions have now been more clearly defined in the manuscript (Line 160 – 180 of manuscript):

"In this study, we introduce an innovating application and design of MGA, applied to a comprehensive U.S. energy system model to assess near-cost optimal decarbonization futures. The model endogenizes technology adoption, allowing for an extensive exploration of technology choices across diverse decarbonization pathways. By incorporating explicit descriptions of the transportation, buildings, power, and industrial sectors, the model accounts for the complex interactions between the major energy sectors. Furthermore, our work extends beyond previous studies in that it accounts for path dependencies resulting from past investments in energy system infrastructure, providing insights into the dynamics of the energy system in later years of the simulations. These features of the modeling effort enable us to better address the questions: What are the characteristics of a wide range of near

cost-optimal pathways that achieve a net-zero energy system in the United States? Are there common themes amongst these pathways, including favored and disfavored technologies, from which we can extract robust insights? Are there correlated decisions in technology adoption that may be particularly informative for policy-making? Through our modeling, we find several consistent trends across the near cost-optimal pathways, including the rapid expansion of solar and wind power generation, substantial reductions in petroleum use, near elimination of coal combustion, and increased end-use electrification. We also observe varying levels of deployment for natural gas, hydrogen, direct air capture of CO2, and synthetic fuels, with important correlations in adoption across some technologies."

3. Furthermore, the rationale for employing energy system optimization models needs strengthening. This should include a detailed explanation of the methods used to analyze path dependencies and near-cost implications.

Text in the manuscript has been added/amended to better motivate the use of energy system optimization models. Line 56 - 57 of manuscript:

"Energy system optimization models (ESOMs) enable the study of energy transitions.[7] These models typically rely on least-cost optimization to inform decision-making, with investment and operational decisions achieving the lowest net present cost. These models determine the optimal deployment of resources, considering existing and new technologies, within a specified time horizon and subject to various constraints. ESOMs can provide insight into crucial decision-making in interlinked systems where analyzing only a single technology or sector in isolation may be insufficient. These models are emerging as the standard in studying macro scale energy systems spanning over multi-decadal time periods.[8] For example, previous studies have used capacity expansion models, a type of ESOM, and explored ranges of fuel and technology options for achieving net-zero CO_2 emissions in the United States by 2050,[9–11] yielding valuable insights into the need for technological flexibility[10] and identifying key challenges and opportunities for decarbonization.[11,12]"

4. Section 2.5 necessitates further development to more effectively explain how carbon emissions are measured. Addressing the complexity of quantifying emissions within interconnected energy systems is crucial, especially concerning the electrification of building appliances, vehicles, and the adoption of solar energy. While the discussion on trade-offs is intriguing, it requires deeper exploration and detail.

Accurate accounting of system-wide emissions is a key advantage of using our comprehensive energy system model. To better clarify the emissions accounting in the model, a new sub-section has been added to the supplementary information (Section S1):

"Emissions Accounting: The model specifies technology-specific pollutant emission factors for all relevant processes in the energy system network. If the model selects a certain process, it incurs emissions proportional to the "emission activity" associated with that process. For example, consider the transportation sector in two scenarios: one with an emissions limit and another without restrictions. In the unrestricted scenario, the model will choose to deploy fossil fuel-based vehicles, which have emission factors measured in 'kt of pollutant/vehicle miles traveled.' The model captures the pollutant burden from using these vehicles, including the upstream emissions associated with the

fuel supply for fossil fuel-based vehicles. In the alternative scenario with an emissions limit, the model is likely to select electric vehicles to meet transportation demand. Although the use of electric vehicles results in no tailpipe emissions, the production of electricity may generate carbon emissions. The model accounts for these emissions as well."

5. Overall, the study should emphasize the uniqueness of its research findings beyond technical modeling. The policy recommendations need to be more closely aligned and integrated with these findings for a cohesive and impactful conclusion.

The following text in the discussion section has been amended to better highlight the uniqueness of the research effort (Line 596 - 610 of manuscript):

"Deterministic energy system optimization modeling can identify least-cost decarbonization pathways, but input assumptions, model representation, and scenario selection constrain insights. Parametric uncertainty methods quantify the impact of uncertain parameters on model outputs. However, diverse near cost-optimal solutions from an ESOM can provide additional insights that cannot be obtained from deterministic modeling alone. Applying MGA to energy systems models provides distinct and diverse alternative pathways that can be missed by parametric assessment methods. In this study, we applied MGA to assess decarbonization pathways for the U.S. energy system, considering path dependencies from early decision-making and the interactions between different sectors of the energy system. Our analysis reveals distinct categories of decarbonization options: those with consistent adoption across pathways, those experiencing universal decline or elimination, technologies with broad outcome distributions, and options highly adopted in only a few pathways. This categorization enhances our understanding of technology dynamics and decarbonization trends."

Reviewer #3 (Remarks to the Author):

This study employs a modelling to generate alternatives (MGA) approach to address the issue of deviations from reality caused by deterministic methods not accounting for uncertainty.

1. Please compare the differences in outcomes, such as the probabilistic profile, between the MGA method and other methods like Monte Carlo analysis, stochastic programming, and robust optimization in addressing parametric uncertainty. Evaluate whether the results from the MGA method are more reliable and its advantages.

The following paragraphs have been reworked to better emphasize the points made by the reviewer:

Line 82 - 118 of manuscript:

"Approaches to address the uncertainty in input parameters include Monte Carlo analysis, stochastic programming, and robust optimization. Monte Carlo analysis involves propagating the uncertainty of one or more input parameters, represented by probability distributions, through the ESOM.[21] Stochastic programming considers numerous uncertain factors in the future and seeks to offer an optimal hedging strategy that informs a single best course of action.[21,22] However, these methods suffer from high computational burdens and require reliable probability distributions for model inputs,[14,22] limiting their effectiveness in ESOMs, particularly when used alongside capacity expansion problems.[22–26] Robust optimization integrates elements from sensitivity analysis, multi-objective optimization, and stochastic programming to produce a set of solutions that gradually become less influenced by the uncertainties associated with input variables. These solutions remain stable and resilient even when facing modeled uncertainties.[14] Unlike stochastic programming, robust optimization cannot provide a unified hedging strategy yet still requires quantification of uncertain model parameters. Further, if knowledge of probability distributions of uncertain inputs is available, this uncertainty can potentially be better captured by other methods.[14]

Structural uncertainties in ESOMs have been shown to lead to dramatic differences in the cost-optimal pathway and real-world energy transitions.[27] Modeling to generate alternatives (MGA) has emerged as a method to mitigate this uncertainty by exploring the near-optimal region to account for unmodelled considerations.[28] MGA produces near cost-optimal solutions which can be maximally different, to allow for more complete consideration of a wide range of alternatives. The solutions from this approach can represent outcomes beyond cost-optimal technology choices, illustrating the potential influence of non-monetary factors such as public acceptance, consumer preferences, and equity on decision-making. Further, MGA alleviates the cognitive biases of the energy modeler and also allows for the inspection of "knife-edge" effects, where small perturbations in the input assumptions can lead to drastically different outcomes.[14,16] The solutions from MGA can be assembled into a portfolio of options and presented to policymakers, giving them insight into making decisions while keeping in mind the interests of multiple stakeholders. These options may be able to capture non-monetary factors without any cognitive biases in a way that deterministic scenario modeling cannot. The applicability of MGA in the context of energy system modeling has been previously demonstrated.[27,30–40]"

2. The paper models different sectors such as electric, buildings, industrial, and transportation sectors using different sources of profiles/inputs settings. The selection of these settings currently lacks consideration of the intersections between sectors and how they interact with each other. Moreover, it should further elaborate on how uncertainties like climate change impact load uncertainty, as well as the uncertainties in the performance of energy sources and end-use devices over long time scales.

We agree with the reviewer that the interaction of the different sectors of the energy system is key to understanding decisions for the energy system as a whole. In fact, this is one of the main strengths of an energy system model. We are grateful to the reviewer for pointing out that these features were not sufficiently highlighted in the previous submission. Text has been added and amended in the manuscript to better highlight this feature.

Line 677 - 684 of manuscript:

"We use the Tools for Energy Model Optimization and Analysis (Temoa), an open-source technology-rich energy systems model. Temoa is structured as a linear problem that can generate the least-cost pathway for energy system development over a user-specified time horizon, subject to system- and user-defined constraints. Temoa represents the energy system as a network of interconnected technologies and commodities. This allows for technology-rich representations of the major sectors of the energy system, which are interlinked through a network. For example, there is competition for energy carriers such as electricity to meet different energy service demands across and within the different sectors."

A new section in the SI discussing the influence of uncertainty from key uncertain input parameters of the model has been added. As part of this section, we conducted additional modeling runs to explore the impact of shifts in the exogenously specified demands, which could be due to climate change impacts, as suggested by the reviewer, on key model outputs. The entirety of this section is not pasted here for brevity but can be accessed in the supplement section S5.

3. In the analysis of near cost-optimal decarbonization pathways, how are technologies selected for application, and what is their contribution to decarbonization? For instance, the reasons for considering battery storage technologies but not thermal storage.

As per the reviewer's suggestion, additional details on how decision-making within the model is now included in the main text. This text reflects the major considerations that can influence endogenous technology choice within the model. Briefly, techno-economic criteria dictate technology choice while respecting the constraints of the model. In the example provided by the reviewer, battery storage would be adopted over thermal storage if the economics, as represented in our model, favor the selection of batteries over thermal storage. In our models, we see a selection of pumped hydro along with batteries to store electricity. We did not have a representation of thermal storage in our database.

Line 692 - 699 of manuscript:

"Installed capacities, associated activities, fuel shares, supply, and end-use technologies are all decision variables optimized in Temoa. Technology choice is based on several techno-economic criteria within the model. The operational characteristics, costs, and lifetimes all influence which technologies

are chosen. The model has perfect foresight across the time horizon, enabling decision-making with the knowledge of future developments like carbon emission targets or changes in fuel price. The optimization of technology choice in end-use technologies is one of the key features of Temoa, similar to the MARKAL TIMES model.[56,57]"

4. Please provide examples of how diverse near cost-optimal scenarios guide energy planning compared to deterministic modeling, and the penetration rates of technologies selected in these scenarios. This is to demonstrate the significance and originality of the research topic.

As per the reviewer's suggestion, additional text highlighting the utility of this modeling effort has been added to the manuscript.

Line 113 - 117 of manuscript:

"The solutions from MGA can be assembled into a portfolio of options and presented to policymakers, giving them insight into making decisions while keeping in mind the interests of multiple stakeholders. These options may be able to capture non-monetary factors without any cognitive biases in a way that deterministic scenario modeling cannot."

REVIEWER COMMENTS

Reviewer #1 (Remarks to the Author):

The authors have thoroughly addressed all the concerns expressed in my first review round. The work has been expanded with additional analyses and Figures when needed and made more transparent, understandable and solid. In particular, the analysis of the effects of an expanded MGA sample size and the sensitivity analysis for parametric uncertainty corroborated the results substantially. The additional points of concern raised by other Reviewers are, in my opinion, also adequately addressed in the revised manuscript. Accordingly, I consider the work in its updated form suitable for publication in Nature Communications.

Reviewer #2 (Remarks to the Author):

The revised manuscript has made significant progress, but there are still areas that need clarification before it can be considered for publication. Specifically, the terms "near cost-optimal net-zero CO2" and relevant related terms need to be clearly defined in the introduction. This will help set a clear context for the study and ensure readers understand the scope and objectives from the outset. Additionally, the connections between Energy System Optimization Models (ESOM) and diverse decarbonization pathways should be elaborated upon beyond the methodology and modeling sections. It is crucial to explain how different models vary in terms of technology and decarbonization methods. Highlighting these differences can address the concern that it is challenging to use a single model to generalize all decarbonization pathways and technology usage. Furthermore, regional differences must be considered, as decarbonization strategies can vary significantly based on geographical, economic, and social factors. I have listed some directions to be considered:

Model and Conceptualization Clarifications

1. Defining clearly near cost-optimal net-zero CO2

2. Clarifying the ESOM models and decarbonization pathways in multidimensional factors:

ESOMs play a crucial role in mapping out various decarbonization pathways. These models help in understanding how different technologies and strategies can be deployed to reduce carbon emissions. It is important to note that different ESOMs may focus on different aspects of the energy system, such as electricity generation, transportation, or industrial processes, and may incorporate varying assumptions about technological advancements, policy measures, and economic factors. So, there are other factors should be considered:

3. Addressing differences in technology and decarbonization methods:

• Technological Focus: Some models may prioritize renewable energy technologies like wind, solar, and hydro, while others might emphasize carbon capture and storage (CCS) or nuclear energy.

• Decarbonization Methods: Approaches can range from increasing energy efficiency and transitioning to low-carbon energy sources to implementing carbon pricing mechanisms and promoting behavioral changes.

• Regional Considerations: Models must account for regional differences in resource availability, infrastructure, economic conditions, and policy environments. For example, strategies suitable for Europe may not be directly applicable to sub-Saharan Africa.

4. Identifying cost-optimization and trade-offs

Purpose of cost-optimization: The primary goal of cost-optimization in the context of achieving net-zero CO2 emissions is to identify the most economically efficient pathways to reduce emissions. This involves minimizing the financial burden on societies while ensuring that the transition to a low-carbon economy is feasible and sustainable.

Trade-Offs considerations:

• Waste: Cost-optimization must consider the potential increase in waste generation from new technologies and find ways to mitigate this impact.

• Justice Issues: Equity and justice are critical considerations. The transition should not disproportionately affect vulnerable populations. Ensuring fair distribution of costs and benefits is essential for social acceptance and sustainability of decarbonization efforts.

Despite the improvements made, this article may still not be suitable for publication in its current form due to the lack of analysis on human behavior and policy-related variables. Incorporating these elements is vital, as they play a significant role in the success of decarbonization strategies. Human behavior influences energy consumption patterns, and policy measures can provide the necessary incentives and regulations to drive change. The article could include:

• Human Behavior: Analysis of how consumer choices, lifestyle changes, and public acceptance impact decarbonization efforts.

• Policy Variables: Examination of existing and potential policies that can facilitate the transition to a low-carbon economy, such as subsidies, taxes, and regulations.

Reviewer #3 (Remarks to the Author):

I have reviewed the revised version submitted by the authors and find that they have adequately addressed my concerns regarding the uncertainty aspects, which has enhanced the robustness of the results. This paper can be accepted in its current form.

Reviewer #3 (Remarks on code availability):

I check the repistories mentioned in the paper Powergenome and Temoa. Detailed instructions have been provided

<u>Response to reviewer comments:</u>

NCOMMS-23-58018: Diverse Decarbonization Pathways Under Near Cost-Optimal Futures

To Whom It May Concern:

We would like to thank the editor and reviewers for their thoughtful and thorough review, and constructive remarks. We are encouraged by the recommendation for publication from Reviewers 1 and 3, and we believe that we have thoroughly addressed Reviewer 2's remaining comments. We have modified the manuscript based on these comments to improve and clarify the text. Please find below detailed responses in **blue** text (with direct quotes from the revised manuscript shown in **bold**, "quoted" and *italic* and text) to the comments and suggestions offered by the reviewers (shown in normal text). All line numbers in our responses correspond to the tracked-changes version of the revised manuscript.

Best regards,

The Authors

REVIEWER COMMENTS

Reviewer #1 (Remarks to the Author):

The authors have thoroughly addressed all the concerns expressed in my first review round. The work has been expanded with additional analyses and Figures when needed and made more transparent, understandable and solid. In particular, the analysis of the effects of an expanded MGA sample size and the sensitivity analysis for parametric uncertainty corroborated the results substantially. The additional points of concern raised by other Reviewers are, in my opinion, also adequately addressed in the revised manuscript. Accordingly, I consider the work in its updated form suitable for publication in Nature Communications.

We thank the reviewer for their insightful comments. Their expertise has greatly enhanced the quality of this manuscript.

Reviewer #2 (Remarks to the Author):

The revised manuscript has made significant progress, but there are still areas that need clarification before it can be considered for publication. Specifically, the terms "near cost-optimal net-zero CO2" and relevant related terms need to be clearly defined in the introduction. This will help set a clear context for the study and ensure readers understand the scope and objectives from the outset. Additionally, the connections between Energy System Optimization Models (ESOM) and diverse decarbonization pathways should be elaborated upon beyond the methodology and modeling sections. It is crucial to explain how different models vary in terms of technology and decarbonization methods. Highlighting these differences can address the concern that it is challenging to use a single model to generalize all decarbonization pathways and technology usage. Furthermore, regional differences must be considered, as decarbonization strategies can vary significantly based on geographical, economic, and social factors.

I have listed some directions to be considered:
Model and Conceptualization Clarifications
1. Defining clearly near cost-optimal net-zero CO2

As per suggestions from the reviewer, we have included the following definitions in the manuscript:

- **Net-zero system (Line 37-39):**
"In net-zero systems, the amount of CO2 emissions released into the atmosphere is balanced by the amount removed through various mechanisms such as carbon capture and storage, reforestation, or technological innovations."
- **Cost-optimal solutions (Line 93-97):**
"MGA produces near cost-optimal solutions which can be maximally different, to allow for more complete consideration of a wide range of alternatives. The solutions from this approach can represent outcomes beyond cost-optimal technology choices, illustrating the potential influence of

non-monetary factors such as public acceptance, consumer preferences, and equity on decision-making."

- **Near cost-optimal net-zero CO_2 (Line 127-130):**

"In the context of this study, near cost-optimal net-zero CO2 futures refer to pathways to achieve net-zero CO2 emissions by 2050 that are close to the lowest possible system cost. These pathways allow for consideration of factors that may be desirable to include but difficult to explicitly model."

2. Clarifying the ESOM models and decarbonization pathways in multidimensional factors:
ESOMs play a crucial role in mapping out various decarbonization pathways. These models help in understanding how different technologies and strategies can be deployed to reduce carbon emissions. It is important to note that different ESOMs may focus on different aspects of the energy system, such as electricity generation, transportation, or industrial processes, and may incorporate varying assumptions about technological advancements, policy measures, and economic factors. So, there are other factors should be considered.

We agree with the reviewer's assessment of ESOMs and have dedicated a paragraph in the introduction to convey these points. The following text has been added/edited to better highlight the reviewer's concerns (Line 47-53):

"Energy system optimization models (ESOMs) enable the study of energy transitions.[7] These models typically rely on least-cost optimization to inform decision-making, with investment and operational decisions achieving the lowest net present cost. ESOMs can determine the optimal deployment of resources, considering existing and new technologies, within a specified time horizon and subject to various constraints. Model designs can vary based on their sectoral representation and assumptions on technology advancements, policy measures, or economic factors."

3. Addressing differences in technology and decarbonization methods:
• Technological Focus: Some models may prioritize renewable energy technologies like wind, solar, and hydro, while others might emphasize carbon capture and storage (CCS) or nuclear energy.

• Decarbonization Methods: Approaches can range from increasing energy efficiency and transitioning to low-carbon energy sources to implementing carbon pricing mechanisms and promoting behavioral changes.

We agree with the reviewer's comments that models designed to express preference for certain technologies or efficiency measures can perhaps inhibit insights. The reviewer will note that a key advantage of our approach is that our model is completely agnostic in technology choice. This is achieved by endogenizing technology choice within the model based on techno-economic characteristics of explicitly defined technologies, engineering constraints and regional demands. The following text is edited on Line 629-632 in the updated manuscript to better clarify this:

"Installed capacities, associated activities, fuel shares, supply, and end-use technologies are all decision variables optimized in Temoa. Technology choice is based on several techno-economic criteria and endogenized within the model."

Additionally, we also clarify that an emissions constraint is imposed in the net-zero run on Line 660-664 of the update manuscript:

"Supplementary Figure S1 shows a flow diagram laying out the main inputs detailed above, and the major outputs analyzed in this work. A deterministic least-cost solution is first obtained by minimizing the total system cost subject to physical, operation, and network constraints as described in above and Supplementary Section S1. The net-zero scenario has an additional emissions constraint driving CO2 to zero by 2050."

• Regional Considerations: Models must account for regional differences in resource availability, infrastructure, economic conditions, and policy environments. For example, strategies suitable for Europe may not be directly applicable to sub-Saharan Africa.

We agree with the reviewer that the spatial resolution of the model is an important consideration in a modeling effort such as this one. We have adopted a nine-region representation of the United States, based on aggregating electric balancing authorities and represent regional differences in resource availability, policy environments and region-specific technology characteristics within these regions. These regions have location-specific data on resource availability and cost. We have added a sentence that clarifies that the solution space is likely to be different for different regions on Line 594-596 of the updated manuscript:

"Additionally, the range of plausible solutions and feasible space is likely to differ for different regions based on local resource availability, behavioral preferences, existing infrastructure and policy environments, among other factors."

4. Identifying cost-optimization and trade-offs
Purpose of cost-optimization: The primary goal of cost-optimization in the context of achieving net-zero CO2 emissions is to identify the most economically efficient pathways to reduce emissions. This involves minimizing the financial burden on societies while ensuring that the transition to a low-carbon economy is feasible and sustainable.
Trade-Offs considerations:
• Waste: Cost-optimization must consider the potential increase in waste generation from new technologies and find ways to mitigate this impact.

The reviewer poses an interesting question that is perhaps currently understudied in the field of macro energy systems research. While there has been a shift in moving beyond least-cost optimization in the last few years, in accounting for equity/environmental justice, material flows of critical minerals, and water use in achieving energy system transitions, much work remains related to accounting for minimizing waste generation from new technologies. The following sentence has been edited to include this observation on Line 591-594 of the updated manuscript:

"Such feasibility analysis should consider material and natural resources constraints, labor implications, supply chain vulnerabilities, climate resilience, environmental justice, waste generation, and energy equity."

• Justice Issues: Equity and justice are critical considerations. The transition should not disproportionately affect vulnerable populations. Ensuring fair distribution of costs and benefits is essential for social acceptance and sustainability of decarbonization efforts.
Despite the improvements made, this article may still not be suitable for publication in its current form due to the lack of analysis on human behavior and policy-related variables. Incorporating these elements is vital, as they play a significant role in the success of decarbonization strategies. Human behavior influences energy consumption patterns, and policy measures can provide the necessary incentives and regulations to drive change. The article could include:
• Human Behavior: Analysis of how consumer choices, lifestyle changes, and public acceptance impact decarbonization efforts.
• Policy Variables: Examination of existing and potential policies that can facilitate the transition to a low-carbon economy, such as subsidies, taxes, and regulations.

The reviewer raises an important concern regarding energy system transitions incorporating justice and equity considerations, human behavior, and policy factors. We acknowledge that these are crucial considerations in decision making related to macro-scale energy system infrastructure.

Policy: We have successfully made extensive efforts to incorporate existing policies in our analyses. For example, Supplementary Section S8 extensively describes how we have included the provisions of the Inflation Reduction Act (IRA) in this work. The effects of the IRA are also discussed in the manuscript: for example, we see that electricity generation from natural gas rebounds in the absence of any provisions once the IRA expires (Figure 2e).

Human behavior, justice and equity: We recognize that while cost is a crucial factor in energy transitions, it is not the sole consideration. The diverse set of near cost-optimal net-zero pathways identified in our study warrants further exploration of their feasibility, particularly in the context of social and behavioral constraints. In fact, this exploration represents a key direction for our research team in future analyses.

Our study presents transition pathways that are technically feasible, as discussed in Line 581 of the updated manuscript. However, we emphasize that technical feasibility does not necessarily equate to implementation viability. Some pathways, despite being technically sound, may be non-viable when factors such as human behavior, justice, and equity are taken into account. Therefore, the set of results presented in this work should be viewed as a collection that defines the technical feasibility space that merits further investigation. To comprehensively assess these options, additional analysis focusing on equity, political feasibility, and other unaccounted-for attributes is necessary. Although performing such a plausibility assessment is beyond the scope of the current work, we acknowledge in lines 579-596 of the manuscript the importance of employing additional analytical tools to identify effective decarbonization pathways.

"The optimization framework used in this paper can help identify the solution space for energy system decarbonization. This solution space contains a diverse array of technically plausible energy pathways. However, technical plausibility is not the same as feasibility. The feasibility of the pathways in the solution space depends on attributes not well-represented in a least-cost optimization framework.[56] For example, consumer behavior and preferences could limit the transition to electric vehicles.[44] In high-penetration renewable systems, tackling the rate of infrastructure buildout, such as the land requirements for wind and solar farms, can be challenging.[57] Furthermore, all the decarbonization pathways in the solution space would require large investments in supporting infrastructure like hydrogen and CO2 pipelines, new transmission lines, and EV charging infrastructure. While the modeling to generate alternatives framework used in this paper can provide valuable insights into the decarbonization solution space, additional analytical tools will be required to identify feasible decarbonization options. Such feasibility analysis should consider material and natural resources constraints, labor implications, supply chain vulnerabilities, climate resilience, environmental justice, waste generation, and energy equity. Additionally, the range of plausible solutions and feasible space is likely to differ for different regions based on local resource availability, behavioral preferences, existing infrastructure and policy environments, among other factors."

Reviewer #3 (Remarks to the Author):

I have reviewed the revised version submitted by the authors and find that they have adequately addressed my concerns regarding the uncertainty aspects, which has enhanced the robustness of the results. This paper can be accepted in its current form.

We thank the reviewer for their insightful comments. We believe their comments have helped improve the clarity and readability of this manuscript.