

# Probabilistic Scenarios Reveal the Impacts of China's Energy System Net-Zero Transition on the Water–Energy–Food Nexus

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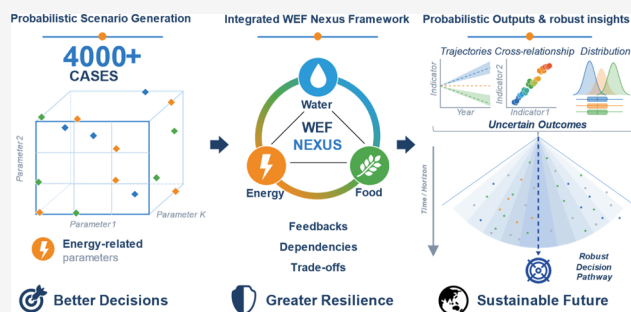
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**ABSTRACT:** China's energy transition toward carbon neutrality tightens interactions across the water–energy–food (WEF) nexus, amplifying systemic uncertainties that are poorly captured in previous assessments. This study develops a probabilistic integrated framework that couples bottom-up models for China's WEF systems with Monte Carlo simulations across technological, policy, and behavioral uncertainty dimensions. By exploring over 4000 uncertainty cases, the framework quantifies not only median trajectories but also the full spectrum of outcomes and the tail risks associated with multidimensional uncertainties. Results indicate large heterogeneity in the probability space: while the median pathway attains deep decarbonization with renewables supplying over 60% of primary energy by 2060, the likelihood of achieving carbon neutrality by 2060 is highly sensitive to carbon capture and storage deployment, the pace of renewable expansion, and cross-WEF-system resource constraints. Early mitigation actions, such as accelerated coal phase-out and rapid scale-up of low-carbon fuels, substantially reduce reliance on negative emission technologies and compresses outcome uncertainty. Sustainability-oriented measures, including water use efficiency improvements and dietary changes, materially relax WEF constraints. These findings deliver actionable diagnostics for policymakers to design decarbonization strategies that reconcile China's net-zero ambitions with long-term WEF sustainability. The methodological framework is transferable to other national contexts where nexus interactions and deep uncertainty govern transition feasibility.

**KEYWORDS:** water–energy–food nexus, Monte Carlo, uncertainty analysis, carbon neutrality, China TIMES, sustainable development, food security, renewable energy



## 1. INTRODUCTION

China's energy transition toward carbon neutrality requires profound transformations in environmental management practices.<sup>1</sup> In the process of climate governance, energy efficiency improves, renewable energy expands, and energy poverty declines.<sup>2</sup> At the same time, the transition interacts closely with food security, water use, and ecosystem protection.<sup>3,4</sup> The energy transition has distinct cobenefits and trade-offs with the sustainable development of the water–energy–food (WEF) nexus.<sup>5</sup> Widespread uncertainties influence technology choices, policy planning, and the feasibility of decarbonization pathways, thereby shaping both the effectiveness and the cost of climate action.<sup>6</sup> A deeper understanding of the connections between climate change mitigation and other environmental policy domains, along with a thorough analysis of how multidimensional uncertainties affect the WEF nexus, can support policymakers in designing integrated decarbonization strategies.<sup>7–9</sup>

The WEF nexus represents one of the domains where social-natural systems are most profoundly affected by the net-zero transition. Given the path-dependent nature of the WEF system, it is urgent to explore synergistic pathways within an

integrated framework that considers the WEF system transition.<sup>10,11</sup> For energy–water nexus, water constraints are becoming a key consideration in energy planning and the selection of transformational technologies for the power and industrial sectors.<sup>12,13</sup> Bottom-up assessments of water system in the agricultural,<sup>14</sup> power,<sup>15–17</sup> and industrial<sup>18,19</sup> sectors typically rely on historical data and lack forward-looking scenario analysis, whereas top-down studies often omit technical details and suffer from sectoral incompleteness. For the energy–food nexus, rising greenhouse gas (GHG) prices incentivize carbon dioxide removal (CDR), whether through afforestation or bioenergy-based technology solutions, leading concerns about food security.<sup>20,21</sup> The trade-offs of biomass supply and forest carbon sinks become progressively significant after carbon peaks.<sup>22,23</sup> Shifts in the dietary structure<sup>24</sup> and

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innovations in land use<sup>25,26</sup> can also substantially influence the costs of the achieving net-zero transition. However, in China, there are few practices linking the land-use model and the energy system model,<sup>27</sup> leaving the cobenefits and trade-offs between the net-zero transition and land-use change insufficiently explored.

Growing research attention is being directed toward the interconnections among multiple systems.<sup>28</sup> Previous assessments indicate that the current configuration of WEF nexus is far from optimal.<sup>29</sup> Retrospective studies employing input–output model<sup>4,30</sup> and structural autoregressive model<sup>31</sup> have quantified the direct and indirect impacts of China's WEF nexus, revealing pronounced trade-offs between food and energy. International integrated assessment model (IAM) team (MESSAGEix,<sup>32</sup> REMIND,<sup>33</sup> AIM,<sup>34</sup> and GCAM<sup>27</sup>) have assessed how climate change mitigation influences the costs and transition pathways for the sustainable development of the WEF system. Nonetheless, substantial gaps persist in understanding the synergistic mechanisms, transition pathways, and enabling policies required to achieve sustainable WEF development under carbon-neutrality scenarios.

Current IAMs follow a scenario-based paradigm, which makes a priori assumptions regarding trends in technological development, consumer behavior, and future policies.<sup>35</sup> In modeling studies, approaches such as multiscenario sensitivity analysis,<sup>36</sup> stochastic programming analysis,<sup>37</sup> multiple quasi-optimal solutions,<sup>38</sup> multisubject behavioral modeling,<sup>39</sup> and Monte Carlo analysis<sup>40,41</sup> are commonly used to quantify uncertainties and their implications for the low-carbon transition. With advances in computational capacity, probabilistic methods have been extended beyond their original applications in technoeconomic models<sup>40</sup> and top-down models<sup>42</sup> to include bottom-up optimization models and IAM frameworks.<sup>43</sup> However, most probabilistic modeling efforts remain confined to individual systems or technologies. The compounded uncertainties within the WEF nexus and the interactions among these uncertainties during the decarbonization of China's energy system remain insufficiently examined.

Here, we propose a novel WEF nexus assessment framework that integrates the bottom-up WEF system modeling with the Monte Carlo simulation. Analysis of thousands of cases reveals that China's carbon neutrality target is ambitious. Multidimensional uncertainties exert substantial influence over transition trajectories, costs, and technology choices. While the net-zero transition creates clear synergies through the diffusion of modern energy and reductions in water withdrawals, the rapid expansion of bioenergy and growing reliance on forest carbon sink may increase competition for land and water resources, with potential implications for food security. These dynamics indicate that carbon neutrality cannot be achieved through energy-sector decarbonization alone but requires coordinated, sector-specific sustainability measures to manage cross-sector risks and enable a smooth and cost-effective net-zero transition.

## 2. MATERIALS AND METHODS

### 2.1. WEF Nexus Assessment Framework

This study developed a probabilistic WEF assessment framework and realized the integration with Monte Carlo analysis to obtain robust insights (Figure S1). The analytical framework consists of three interconnected models: an energy–environment–economy model (China Integrated MARKAL-EFOM System version 2.0, China

TIMES 2.0), a land-use model (Global Biosphere Management Model-Global Forest Model, GLOBIOM-G4M), and a water model (Community Water Model, CWatM).

China TIMES 2.0<sup>10,44</sup> is a national bottom-up energy–environment–economy optimization model developed by Tsinghua University, building on China TIMES<sup>41,45,46</sup> and China MARKAL.<sup>47–49</sup> The model uses 2019 as the base year, covers 2019–2100, and calibrates 2019–2023 data to official statistics. The model portrays the whole energy chain from energy extraction, transformation, distribution, and end use, covering energy supply,<sup>50,51</sup> industry,<sup>52,53</sup> building,<sup>54</sup> transportation,<sup>55</sup> and agriculture. The model includes more than 2000 technologies and multiple supply curves for key energy activities. Further details are provided in Notes S1 and TIMES documentation ([https://github.com/etsap-TIMES/TIMES\\_Documentation](https://github.com/etsap-TIMES/TIMES_Documentation)).

GLOBIOM<sup>56–58</sup> is a model developed by IIASA to analyze agriculture, forestry, biomass development, and land-use change. It is a partial equilibrium model, solved recursively and dynamically with a base year of 2000 and a simulation period up to 2100, capable of processing gridded data with a 0.5° accuracy. The model evaluates food, wood, and biomass production patterns at a global scale, focusing on land-use change in six land cover categories (cropland, grassland, rotational plantations, managed forests, unmanaged forests, and natural vegetation). To provide a more detailed representation of the forestry system, GLOBIOM is linked to G4M, enabling the estimation of CO<sub>2</sub> emissions and removals from forestry activities in managed forests. Details can be found at the official website (<https://globiom.org/>).

CWatM<sup>59,60</sup> is an open-source model developed by IIASA to study future patterns of water supply and demand in relation to socioeconomic development and climate change. The model integrates water demand for agriculture, building, energy supply, and the natural environment, considering the energy needs associated with water supply. CWatM model divides the land cover into six categories (forest, grassland, cropland, rice paddies, urban, and water surface). Each land cover type is represented by three soil layers, which in turn are associated with distinct soil processes. It is capable of dynamically simulating the water quantity of groundwater, lakes, reservoirs, and rivers. In this study, hydrologic dynamics are simulated for 2015–2100 at a 0.5° spatial resolution and monthly temporal resolution. The model and documentation are available online (<https://cwatm.iiasa.ac.at/>).

To realize the connection between China TIMES 2.0 and GLOBIOM-G4M, this paper uses the biomass supply and GHG emissions as the coupled variables. Biomass supply prices and GHG prices endogenously determined by the energy system model are used as inputs to the land-use model, which feeds back land-sector-optimized biomass supply potentials to the energy model as constraints, while simultaneously outputting land-sector transition dynamics, including food supply and demand, biomass supply, AFOLU emissions, and land-use change patterns. Land system feedback mainly affects the feasibility and cost of bioenergy, and bioenergy with carbon capture and storage (BECCS) deployment in China TIMES. This, in turn, will affect the balance between forest carbon sinks and bioenergy-based CDR technologies. Specifically, the energy model includes disaggregated biomass supply technologies (e.g., agricultural residues, forestry residues, and dedicated energy crops) that interface directly with the land model. To reduce computational burden and enable large-scale uncertainty analysis, a GLOBIOM-G4M emulator is integrated into China TIMES 2.0. The emulator comprises 84 preoptimized land-sector pathways based on combinations of seven biomass price (0, 3, 5, 8, 13, 30, and 60 USD/GJ) and 12 GHG price parameters (0, 10, 20, 50, 100, 200, 400, 600, 1000, 1500, 2000, and 3000 USD/tCO<sub>2</sub>eq), which are linearly combined during energy system optimization to represent land-sector transition dynamics.

CWatM is soft linked to China TIMES 2.0 and GLOBIOM-G4M. China TIMES 2.0 provides water demand projections for the power and industrial sectors to CWatM, while GLOBIOM-G4M supplies information on cultivated area, irrigated area, and land-use patterns.

CWatM independently estimates building-sector water demand based on downscaled population data, simulates water availability by source, consumption and withdrawals by sector, and feeds back region-specific water availability and water supply costs to both China TIMES 2.0 and GLOBIOM-G4M, which affect the feasibility and competitiveness of energy technologies such as hydro, thermal power, hydrogen production, BECCS-related options. Within the energy model, we explicitly represent water supply technologies (e.g., surface water, groundwater, seawater desalination, and reclaimed wastewater). Each power and industrial technology is assigned water withdrawal and consumption coefficients, while water demand in the buildings sector is calibrated based on per-capita water use assumptions.

### 2.2. Scenario Design and Assumptions

To assess the implications of the net-zero transition for WEF nexus, this study develops a structured set of reference and mitigation scenarios. A reference scenario (REF) is constructed by incorporating only energy and climate policies enacted by 2022 (Table S1), together with China's carbon peaking target. Additionally, we embed key land and water policy constraints in the model to ensure a realistic representation of China's land and water system. These include a monotonic decline in traditional biomass use; population-scaled cropland protection and grain production targets; mandated reductions in industrial water intensity and water use per unit of GDP by 2025 and 2030; expansion of desalination and wastewater treatment capacity; a post-2025 decline in groundwater extraction; and seasonal ecological flow requirements that reserve fixed shares of streamflow in wet and dry periods.

Building on this baseline, two net-zero scenarios are designed, differentiated by the timing of mitigation onset: a planned transition starting in 2030 (CN60) and an early action scenario initiating in 2025 (CN60E). To explore net-zero pathways that are compatible with long-term WEF sustainability in China, a parallel set of sustainability-enhanced scenarios was developed. These include a sustainability reference scenario (REF-SDG) and two net-zero scenarios with integrated sector-specific sustainability measures (CN60-SDG and CN60-SDGE), which aim to identify net-zero transition pathways that jointly support climate mitigation and WEF sustainable development. Table 1 summarizes the key assumptions across the scenarios.

The sustainability scenarios introduce policy measures in WEF systems that are consistent with sustainable development goals (SDGs) or proxy indicators. More detailed information can be found in Table S2.

**Table 1. Comparison of Scenario Assumptions**

| scenario assumption                                                         | REF | REF-SDG | CN60 | CN60-SDG | CN60E | CN60-SDGE |
|-----------------------------------------------------------------------------|-----|---------|------|----------|-------|-----------|
| energy and climate policies issued by 2022                                  | ✓   | ✓       | ✓    | ✓        | ✓     | ✓         |
| fossil fuel and industrial (FFI) CO <sub>2</sub> emissions peak before 2030 | ✓   | ✓       | ✓    | ✓        | ✓     | ✓         |
| net-zero FFI CO <sub>2</sub> emissions by 2060                              |     |         | ✓    | ✓        | ✓     | ✓         |
| monotonous decline in CO <sub>2</sub> emissions after 2030                  | ✓   | ✓       | ✓    | ✓        | ✓     | ✓         |
| Early retirement allowed after 2030                                         |     |         | ✓    | ✓        | ✓     | ✓         |
| price elasticity of demand                                                  |     |         | ✓    | ✓        | ✓     | ✓         |
| continuing the REF/REF-SDG pathway to 2025                                  |     |         |      |          | ✓     | ✓         |
| continuing the REF/REF-SDG pathway to 2030                                  |     |         | ✓    | ✓        |       |           |
| sustainability measures                                                     |     | ✓       |      | ✓        |       | ✓         |

### 2.3. Uncertain Scenario Generation Approach

To address multidimensional uncertainty, we propose a probabilistic scenario-generation approach. Parameter combinations are stratified from prior distributions using Latin Hypercube Sampling.<sup>61</sup> For each sampled parameter set, the model is optimized to determine transition dynamics, effectively implementing a Monte Carlo-based analysis of system responses.<sup>41,43,62,63</sup> The resulting distributions are then analyzed to characterize the uncertainty in the outcomes.

Our uncertainty framework explicitly incorporates key parameters spanning resource endowments, energy supply, demand dynamics, and climate policy dimensions. Cumulative emission constraints represent the most critical determinant of decarbonization pathways and WEF nexus impacts. For renewable technologies, we focus on wind, solar, and storage costs and resource potentials, as prior literature identifies these as China's primary decarbonization pillars. Nuclear power uncertainties encompass both cost trajectories of domestically commercialized Gen-III and emerging Gen-IV reactors and potential policy shifts regarding inland siting, which could substantially alter geographic flexibility and water-cooling demands. Hydrogen production costs are included due to their pivotal role in determining end-use sector decarbonization pathways. BECCS costs feature prominently as this technology constitutes the primary negative emission source, critically affecting feasibility of carbon neutrality. Finally, demand price elasticity parameters capture consumer responsiveness to energy pricing signals, representing behavioral dimensions in end-use sectors.

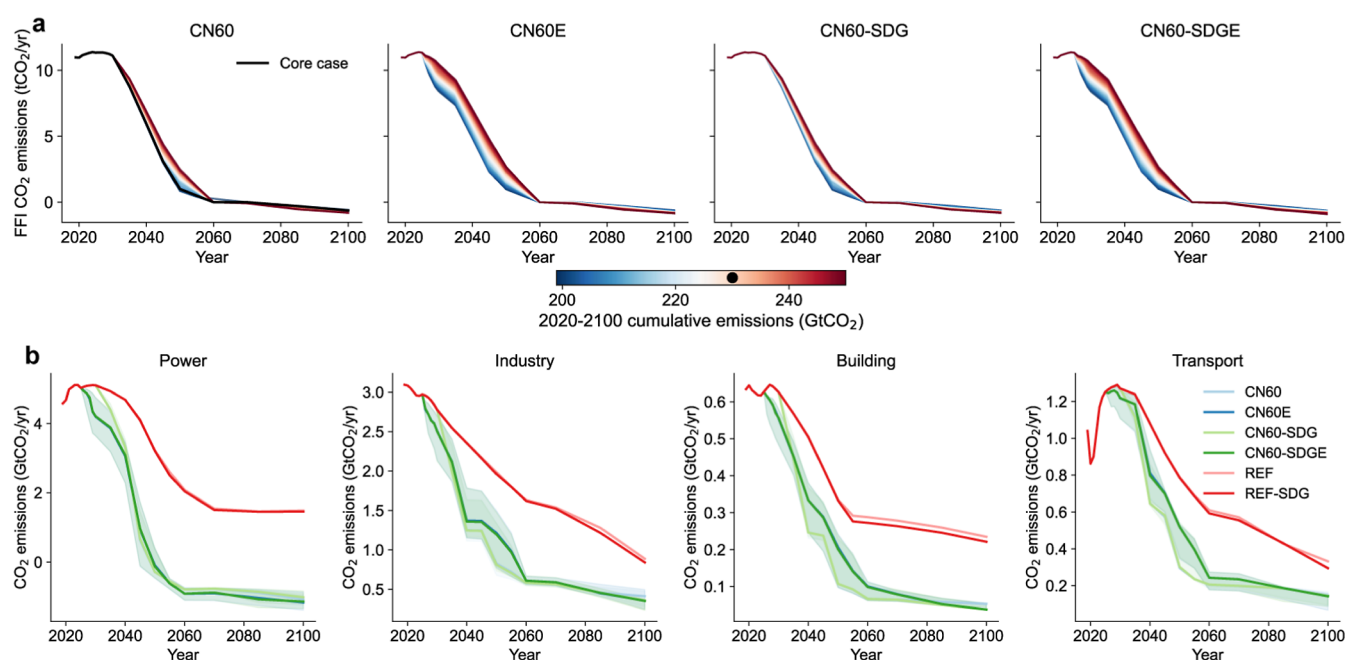
All uncertainty cases are generated as perturbations of the core cases, whose parameter assumptions are listed in Tables S3–S5. The uncertainty ranges were designed to represent plausible deviations from the core case assumptions rather than precise predictive probability distributions. Technology cost uncertainty was represented by log-normal perturbations spanning 70%–143% of the core-case values because future technology costs are non-negative and tend to evolve multiplicatively. The range was selected by benchmarking against the spread of recent clean-technology cost projections.<sup>64</sup> Capacity growth rates<sup>65,66</sup> and energy demand price elasticities<sup>67</sup> were perturbed using normal distributions within ±30% of the core assumptions to reflect uncertainty in deployment feasibility and demand response. A uniform range of 200–250 GtCO<sub>2</sub> was applied to cumulative fossil-fuel and industrial (FFI) CO<sub>2</sub> emissions over 2020–2100 to cover the median outcomes of multiple carbon allowance allocations<sup>68</sup> consistent with both 1.5 and 2 °C temperature targets. The full list of uncertain parameters, distributions, ranges, and supporting references is provided in Table S6. The sampled distributions used in this study should be interpreted as a structured representation of plausible uncertainty scenarios rather than as predictive probability distributions. In this paper, cases with marginal abatement costs (MACs) exceeding 800 USD/tCO<sub>2</sub> in any year are considered economically infeasible and discarded.

## 3. RESULTS

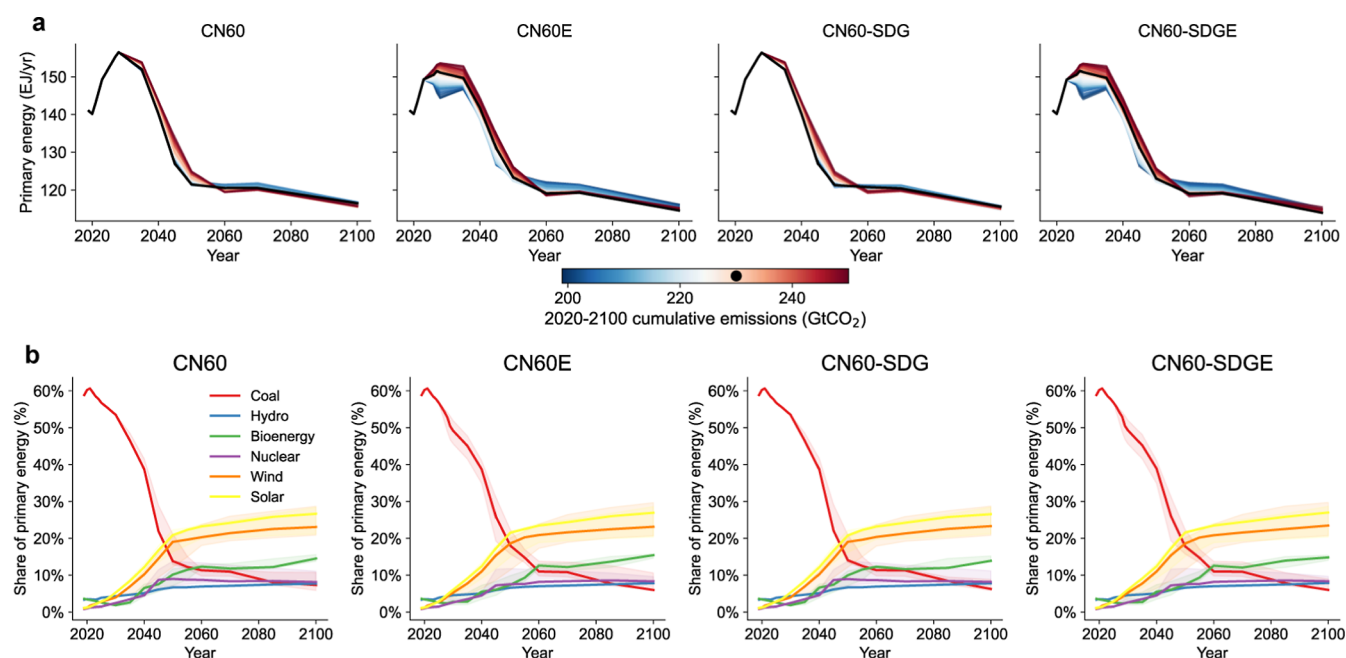
### 3.1. Carbon Emissions and Removals

Figure 1 presents FFI CO<sub>2</sub> mitigation pathways under perturbations of the key uncertainty parameters. Given the dual constraints of net-zero emissions and cumulative carbon emissions, FFI emissions under net-zero scenarios declined sharply between 2030 and 2060. In the early action scenario, FFI CO<sub>2</sub> emissions are estimated to be projected to decline by 17% (8%–27%) within five years following their peak. As 2060 approaches, the net-zero constraint narrows the uncertainty range of the residual emissions. Beyond 2060, however, the spread of negative emissions widens considerably. This highlights a key trade-off for China: accelerate near-term mitigation to constrain cumulative CO<sub>2</sub> emissions or increase reliance on long-term CDR.

The power sector is the largest source of CO<sub>2</sub> emissions. In all scenarios, decarbonization of the power sector precedes



**Figure 1.** FFI CO<sub>2</sub> emissions in China. (a) CO<sub>2</sub> emissions by scenario. (b) CO<sub>2</sub> emissions by sector.

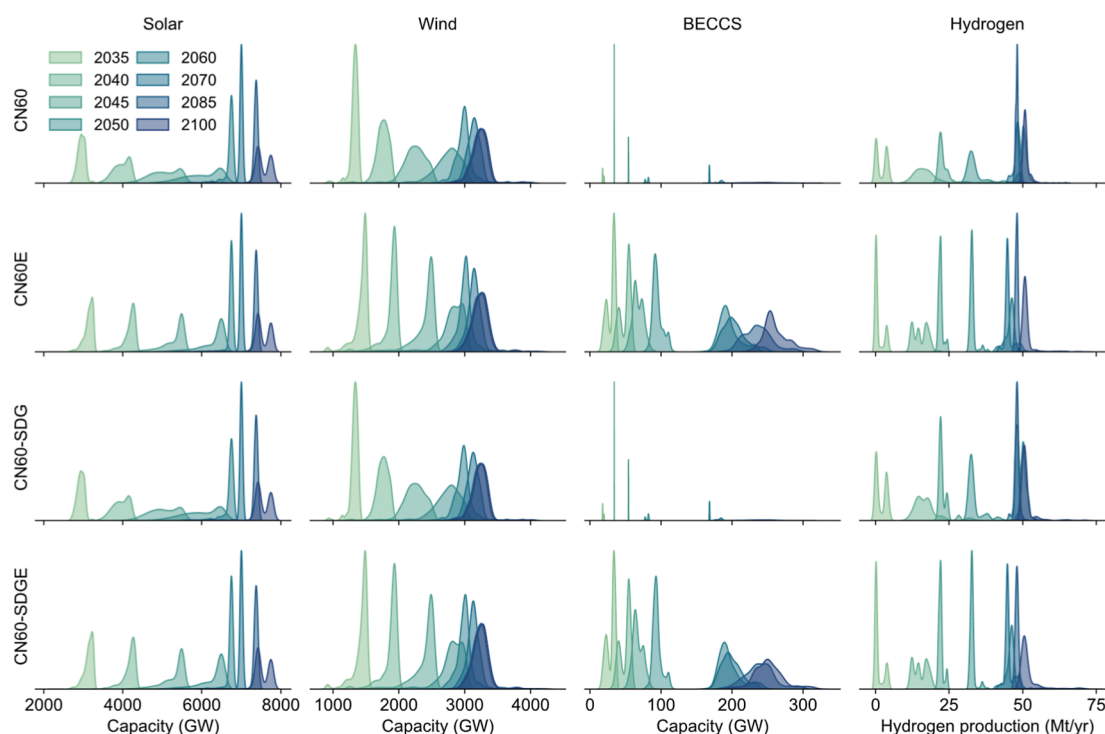


**Figure 2.** Primary energy supply in China. (a) Primary energy supply by scenario. (b) Primary energy supply by fuel. More details can be found in Figures S5–S6.

economy-wide net-zero emissions. In the CN60 scenario, more than half of the cases require net-negative emissions by 2050, whereas in the CN60E scenario, approximately one-fifth reach net-negative emissions as early as 2045. By 2100, biomass availability constraints limit the power sector's potential for net-negative emissions to 0.9–1.4 GtCO<sub>2</sub>. Promoting the early retirement of thermal power units commissioned after 2010 by ten years drives a pronounced decline in power-sector emissions.

While emissions from the industrial and building sectors have already peaked, those from the transportation sector are not expected to peak until ~2030. Industrial sector emission

abatement will depend heavily on low-carbon fuels as well as carbon capture, utilization, and storage (CCUS), particularly between 2040 and 2060. In the building sector, emission reductions will be driven by building envelope retrofits, electrification, and shifts in public behavior, leaving residual emissions of 100–230 MtCO<sub>2</sub> by 2050. The transportation sector is currently experiencing a decelerating rate of emission growth, as rapid electric vehicle development partially offsets rising mobility demand. Residual emissions are projected to arise primarily from aviation and marine transport, with deep decarbonization being contingent on biofuels and hydrogen-derived fuels.



**Figure 3.** Probability density distribution of solar power capacity, wind power capacity, BECCS capacity, and hydrogen production by scenario by year. More details can be found in [Figures S7–S13](#).

[Figure S2](#) shows trajectories of CO<sub>2</sub> capture via CCUS. Large-scale CCUS deployment is projected to begin after 2030, with annual captured CO<sub>2</sub> reaching 0.4–0.7 GtCO<sub>2</sub> by 2040. Under the early action scenario, this range widens to 0.3–1.4 GtCO<sub>2</sub>. By 2060 and 2100, captured CO<sub>2</sub> increases to 1.6–1.8 GtCO<sub>2</sub> and 1.6–2.0 GtCO<sub>2</sub>, respectively.

BECCS in the power sector accounts for most of the CDR through engineering-based solutions. Cumulative carbon emissions and costs are the primary drivers shaping the BECCS deployment. Furthermore, BECCS exhibits a substitute relationship with wind, solar, and hydrogen. The CN60E scenario, which includes a broader portfolio of decarbonization options, yields a wider distribution of BECCS deployment compared to CN60. Retrofit-capable coal-fired units are prioritized for BECCS integration, supplemented by a limited number of new precombustion BECCS facilities. In contrast, under biomass-constrained conditions, fewer plants would be retrofitted with CCUS, resulting in captured CO<sub>2</sub> of below 0.3 GtCO<sub>2</sub> by 2060.

CO<sub>2</sub> captured in the industrial sector originates primarily from iron making, cement production, and ammonia synthesis. High capital and operational costs associated with substituting conventional processes with hydrogen- or electricity-based alternatives sustain significant technical and economic uncertainty surrounding industrial CCUS deployment through 2050. Beyond 2060, advances in hydrogen-based ironmaking technologies are projected to reduce the reliance on CCUS, thereby lowering both total captured volumes and the associated uncertainty ranges.

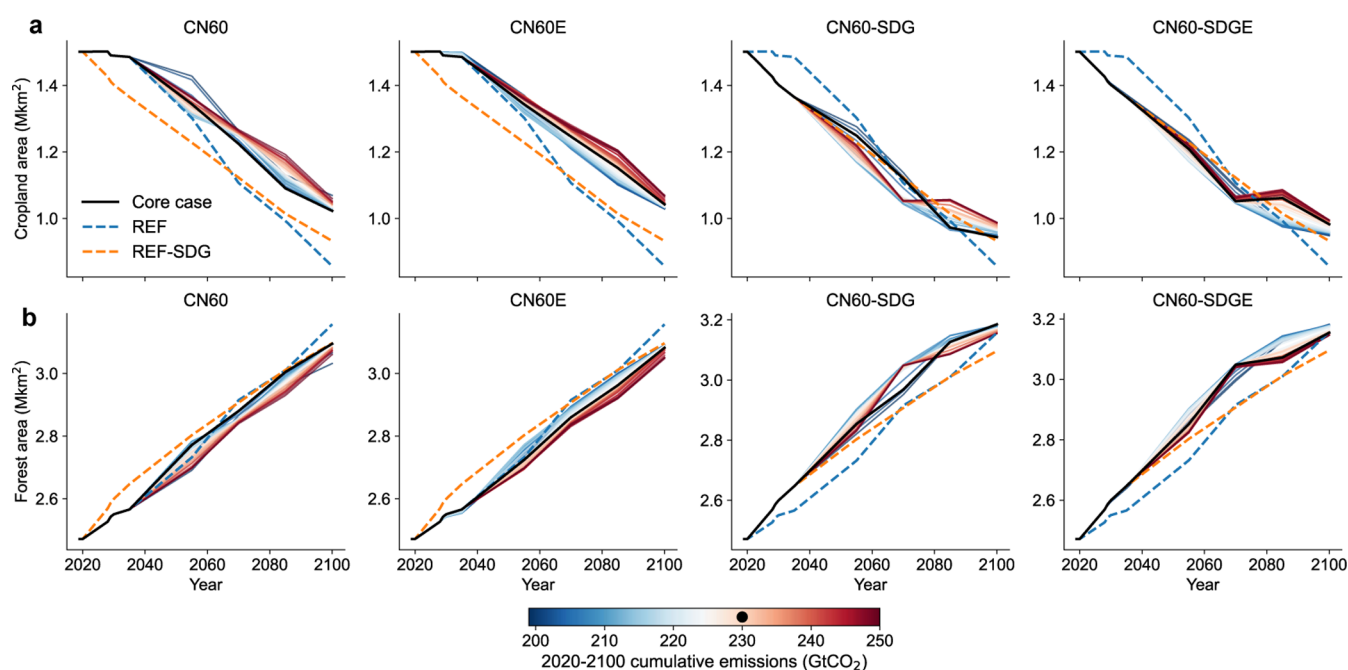
Negative emissions play a critical role from 2060 onward. Thanks to integrated WEF nexus optimization, the dynamics of how engineering- and nature-based solutions contribute to negative emissions can be explored. Engineering-based solutions (primarily BECCS) deployed in power generation and hydrogen production deliver 0.97–1.45 GtCO<sub>2</sub> of negative

emissions in 2060, rising to 1.14–1.80 GtCO<sub>2</sub> by 2100. Nature-based solutions, including afforestation and forest management, contribute an additional 0.58–0.66 GtCO<sub>2</sub> of negative emissions by 2060, increasing modestly to 0.60–0.75 GtCO<sub>2</sub> by 2100. A significant trade-off emerges between these two approaches, intensifying as the overall negative emission demand grows. On average, each additional unit of BECCS-driven removal displaces 0.01 and 0.14 units of the forest carbon sink by 2060 and 2100, respectively. This substitution effect is markedly stronger in scenarios without an early climate action. Under the CN60 and CN60-SDG scenarios, the displacement ratios reach 0.33 and 0.49 in 2060. Although the trade-off weakens somewhat by 2100, it remains substantially higher than that in the early action scenarios.

### 3.2. Energy Transition and Key Technology Deployment

As illustrated in [Figure 2](#), all scenarios show a consistent trajectory of gradually declining fossil fuel consumption and a substantial expansion of renewable deployment, which forms the backbone of China's net-zero transition. Under the CN60E scenario, primary energy supply peaks at 153 EJ around 2028 and declines to 116–125 EJ by 2060. The share of renewables rises from 10% in 2020 to 25% (20%–28%) by 2035 and further to 64% (60%–66%) by 2060. Coal's contribution drops sharply from 54% in 2030 to just 11% by 2060. Driven by sustainability measures, traditional biomass combustion declines before 2035, then modern biomass energy gains attraction, resulting in a combined biomass share of 12%–13% by 2060. This shift reflects accelerated electrification, stringent coal controls, and targeted support for modern bioenergy under enhanced climate ambition.

[Figure 3](#) presents the probability density distributions for key low-carbon technologies: solar, wind, BECCS, and hydrogen. By 2060, solar (5.6–6.8 TW) and wind (2.6–3.5 TW) are projected to dominate the power system. However,



**Figure 4.** Cropland and forest area by scenario. (a) Cropland. (b) Forest.

their deployment trajectories remain highly uncertain, shaped by factors including cumulative carbon emissions, investment costs, resource availability, and the pace of technology rollout. Solar expansion is particularly sensitive to the deployment growth limit, while wind capacity shows greater responsiveness to capital cost variability. This uncertainty propagates directly into storage requirements. Battery storage is expected to provide 15% of the total annual generation by 2060, with capacity ranging narrowly between 1104 and 1275 GWh, scaling almost linearly with wind and PV capacity. In contrast, mechanical storage exhibits broader uncertainty, as its deployment depends on a more complex set of drivers: capital cost, variable renewable penetration, PV and wind economics, and cumulative emission constraints.

Hydrogen deployment is concentrated before 2060, primarily driven by tightening climate targets. Its scale exhibits a strong, near-exponential relationship with both cumulative carbon constraints and annual CO<sub>2</sub> emissions, underscoring its role as a flexible compliance instrument in deep decarbonization pathways. Hydrogen energy final consumption is expected to reach 40–53 MtH<sub>2</sub> by 2060. In China, the hydrogen supply will be dominated by three pathways: grid-connected water electrolysis, off-grid renewable-powered water electrolysis, and BECCS-based production. While hydrogen use in transport remains limited through 2030, its highest impact applications lie in hard-to-electrify sectors, particularly hydrogen-based ironmaking, green ammonia, and green methanol.

Although supply-side decarbonization is essential, demand-side transformations are equally critical. Final energy consumption peaks around 2030, making electrification and hydrogen central to efficiency gains and emission abatement. Under the CN60E scenario, the electrification rate reaches 54%–58% by 2060. Transport leads this shift, rising from 5% in 2020 to 46% by 2060, followed by buildings, where electrification doubles to 75% by 2060, driven by electric space heating (62% of heating) and electric stoves (83% of cooking demand).

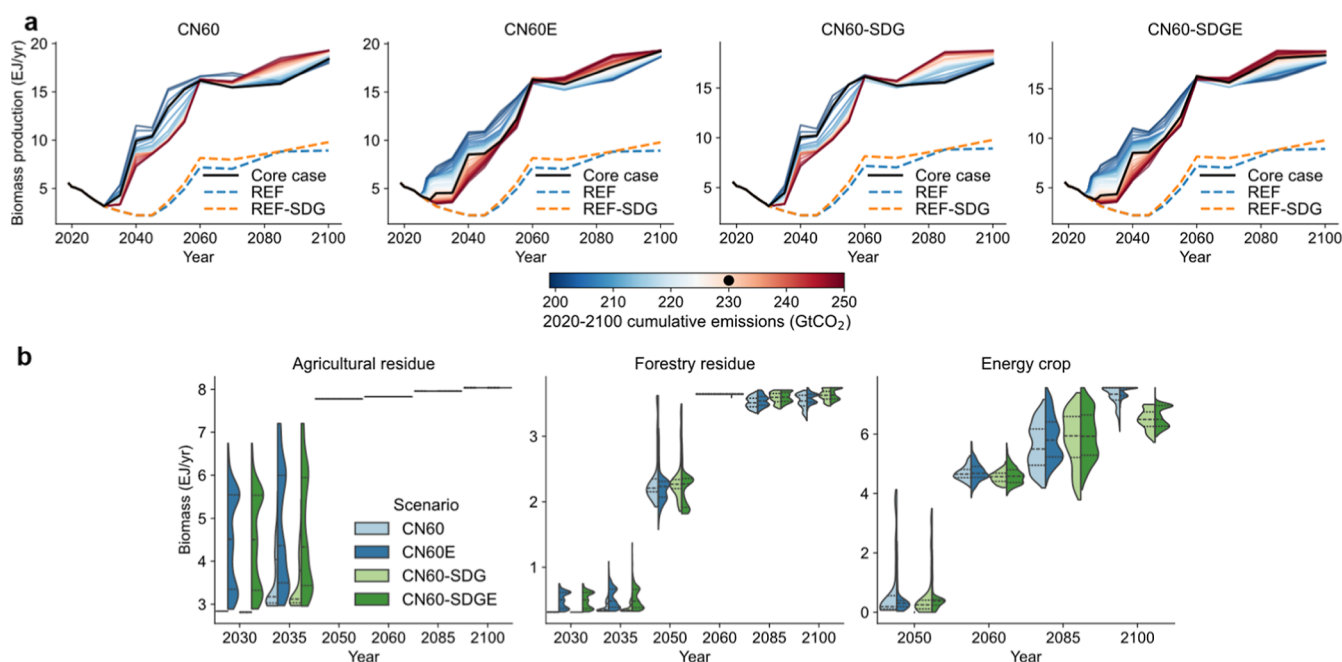
Changes in production and consumption patterns further shape demand (Figure S3). By 2060, under the CN60 scenario, marked declines are observed in energy-intensive output compared to the REF scenario, with cement dropping by 7.5%, steel by 12%, ammonia by 15%, and aluminum by 15%. Domestic freight turnover falls by up to 8%, with hard-to-abate aviation and shipping declining by up to 15%. As carbon neutrality nears, demand changes become increasingly uncertain, driven by stringent climate policies that raise energy costs in high-emission sectors, reducing demand due to elevated prices, and by growing availability of low-carbon alternatives, which heighten demand elasticity. While greater elasticity suppresses energy use and emissions, it may entail welfare losses and significant social costs.

### 3.3. Land and Water Systems' Synergistic Transformation

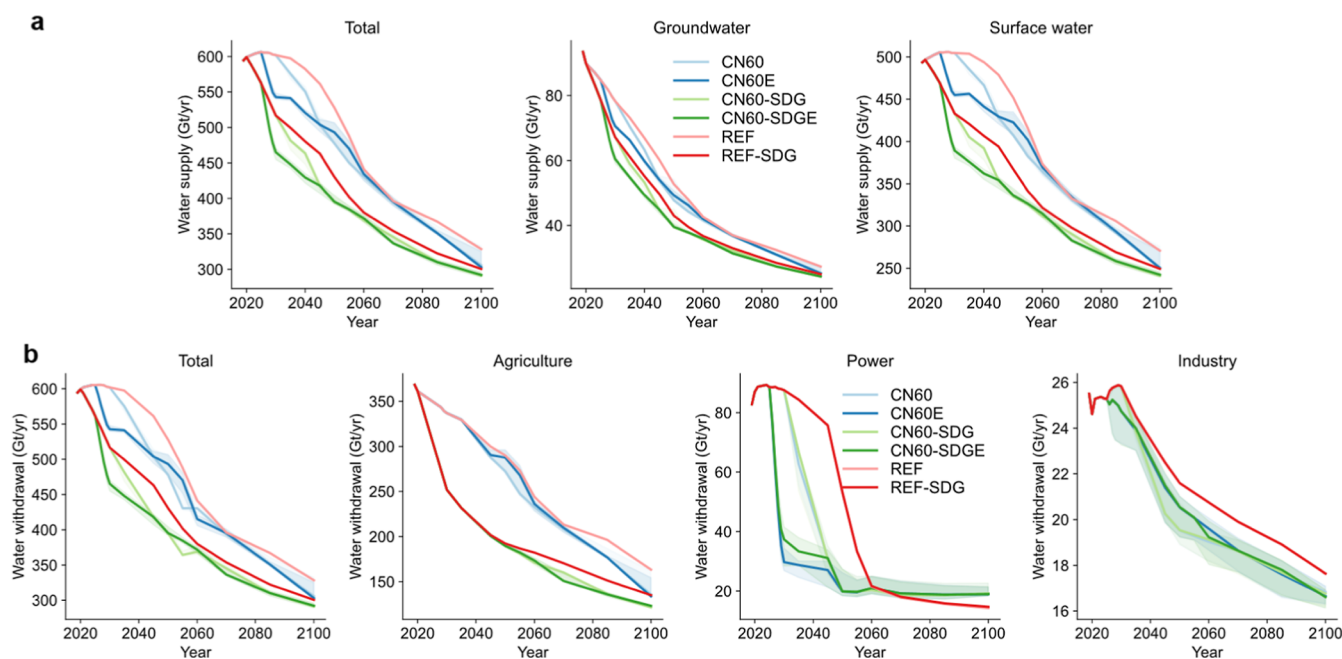
Land system is deeply intertwined with China's net-zero transition. It supplies biomass feedstocks essential for bioenergy and BECCS while simultaneously acting as a major source of GHG emissions and a critical carbon sink. This duality not only creates key trade-offs between energy security, food production, biodiversity, and climate mitigation but also enables powerful synergies when managed coherently.

Land-use patterns will evolve gradually alongside socioeconomic development (Figure 4). In non-SDG scenarios, the pathways under the CN60 scenario closely track those of the REF scenario until 2045. However, the large-scale deployment of dedicated energy crops introduces significant land-use uncertainty thereafter. By 2060, cropland area exceeds 1.2 Mkm<sup>2</sup>, while forest area ranges from 2.73 to 2.80 Mkm<sup>2</sup>. Over 2020–2100, low cumulative-emission cases expand forest cover by 0.1 Mkm<sup>2</sup> relative to high-cumulative-emission counterparts, underscoring the pivotal role of nature-based solutions in achieving net zero.

Under SDG scenarios, enhanced land, food, and forest system measures substantially accelerate afforestation. By 2060, the forest area reaches 2.90–2.97 Mkm<sup>2</sup>, exceeding non-SDG scenarios by 1.7 Mkm<sup>2</sup>. This demonstrates how sustainable



**Figure 5.** Biomass production in China. (a) Biomass production by scenario. (b) Biomass production by source.



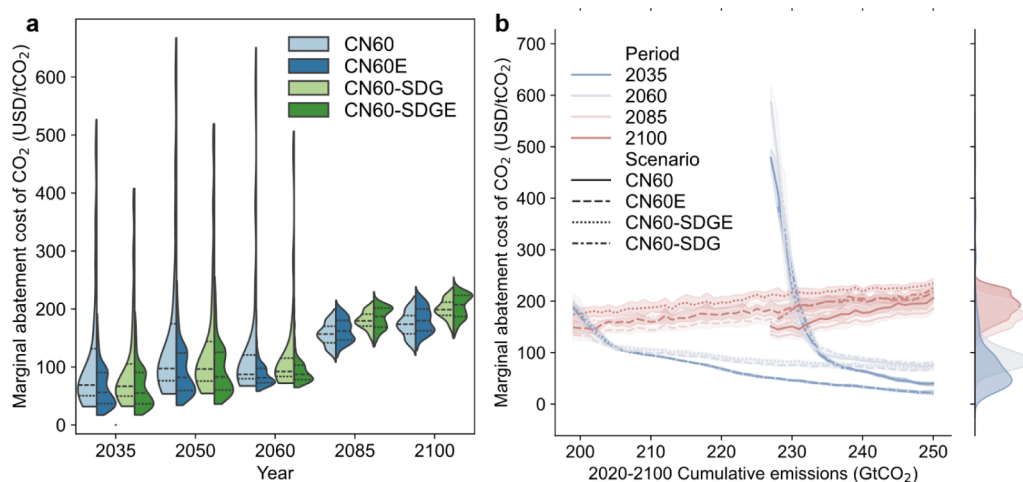
**Figure 6.** Water supply and withdrawal patterns in China. (a) Water supply by source. (b) Water withdrawal by sector. More details can be found in Figures S15–S16.

development priorities can amplify climate mitigation cobenefits while alleviating land-use conflicts.

Biomass serves as the feedstock for BECCS; its cost and availability determine the potential for future negative emissions and the upper limit of residual emissions under a net-zero emission scenario. As shown in Figure 5, biomass production follows a U-shaped trajectory, declining to a minimum around 2030 before rising to more than three times its 2020 level by 2060. After 2050, agricultural and forestry residues become insufficient to meet the growing bioenergy demand, triggering the large-scale deployment of dedicated energy crops. This shift introduces significant land-use

uncertainty, as the scale of energy crop cultivation directly reflects uncertain future bioenergy requirements.

Early climate action plays a crucial role in maximizing land system synergies. Under the SDG scenarios, expanded forest areas due to restrictions on development in biodiversity hotspots not only enhance carbon sequestration but also slightly increase the supply of forestry residues, enabling higher sustainable bioenergy yields without extensive cropland conversion. Similarly, accelerating biomass industry development prior to 2030 under the CN60E scenario reduces reliance on energy crops later in the century, thereby minimizing land competition and preserving ecosystem integrity. In contrast,



**Figure 7.** Marginal abatement cost of CO<sub>2</sub>. (a) Probability density distribution of the marginal abatement cost of CO<sub>2</sub>. (b) Distributional relationship between the marginal abatement cost of CO<sub>2</sub> and cumulative emissions. More details can be found in Figure S4.

delayed action defers biomass mobilization, leading to sharper, more land-intensive energy crop expansion after 2050.

Despite these divergent pathways, biomass consumption converges across all scenarios after 2060, driven by persistent negative emission demands. Nevertheless, the timing of action critically determines whether land-use change amplifies environmental trade-offs or unlocks cobenefits for climate, biodiversity, and food security.

Figure S14 shows the per-capita daily calorie intake and the share of animal-source foods. Under the CN60 scenario, plant-based calories remain stable through 2035, while animal-source intake rises by 22% relative to 2019. The total per-capita consumption peaks in 2035 but then declines steadily, falling to 2700 kcal·capita<sup>−1</sup>·day<sup>−1</sup> by 2100. After 2035, feed-food competition increasingly constrains livestock production, capping animal-source calories at just over 26% of total intake.

Critically, without deliberate shifts toward more sustainable diets, future calorie availability will decline sharply, driven by land constraints, bioenergy demand, and climate mitigation pressures. Under the CN60-SDG scenario, we set the proportion of animal-sourced foods to be below 15% by 2060. The result shows that the animal-source calorie intake drops by 17% by 2035, even as the total intake climbs 14%, and by 2060 animal-source intake decreases to 72% of 2019 values with the total intake sustaining above 3000 kcal·capita<sup>−1</sup>·day<sup>−1</sup>.

Water is used extensively in agriculture, thermal power generation, hydrogen production, BECCS, and industrial manufacturing. Under water constraints, water-saving technologies and seawater desalination technologies have advanced. As shown in Figure 6, the water withdrawals exhibit a steady downward trend, decreasing to 420–440 Gt by 2060 and further declining to 300–330 Gt by 2100. Under the CN60 scenario, water withdrawals could be reduced by 60 Gt compared with the REF scenario during the 2030–2050 period. However, after 2060, this gap narrows, as coal-fired power plants in the REF scenario are also phased out. The CN60-SDG scenario, in which the rapid scale-up of water-efficient irrigation is achieved in the near term, will reduce water withdrawals by 100 Gt compared to the REF scenario by 2035. Although the gap between CN60 and CN60-SDG gradually narrows thereafter, the two scenarios still differ by approximately 10 Gt by 2100.

In terms of water sources, surface water maintains an approximately 83% share of the total water supply, while groundwater extraction declines from the current 15% to approximately 10% by 2060. Under the CN60 scenario, groundwater extraction is reduced to less than 80 Gt by 2030, essentially resolving the issue of excessive groundwater extraction. Under the SDG scenario, this issue is resolved even earlier by 2025.

Sectorally, agriculture dominates water withdrawals, with eco-friendly irrigation relying on the expanded water-saving infrastructure. By 2060, agricultural water withdrawals decrease steadily to 228–240 Gt by 2060 under CN60 and to 172 Gt under CN60-SDG. Power and industrial sectors' water conservation closely ties to the energy transition. Compared to the CN60 scenario, net-zero transitions start earlier under the CN60E scenario, resulting in water use reductions: by 2035, even the highest water use case in CN60E (25–30 Gt) is 25 Gt lower than the lowest water use case in CN60 (55–65 Gt). Under the CN60 scenario, recirculating cooling thermal power plants dominate in 2019, accounting for 67% of the capacity, while air-cooled units represent 18%. The share of air-cooled units increases to 21% by 2030, 24% by 2060, and 29% by 2100 (Figure S17).

Despite these improvements, the reductions in water withdrawals are not sufficient to achieve water-related SDG targets. After 2060, the power sector's water consumption in mitigation scenarios tends to increase due to the deployment of water-intensive technologies like BECCS and CCUS, indicating a trade-off between BECCS development and water conservation. Industrial water withdrawals continue to fluctuate downward before 2060, reaching 18–19 Gt by 2060, but cases with lower cumulative emissions experience faster energy efficiency upgrades before carbon neutrality, driving industrial water conservation. After carbon neutrality, however, these cases see higher water consumption due to the increased use of CCUS and other water-intensive technologies. Therefore, while the ongoing energy transition has already produced notable improvements in water resource management, additional actions are urgently needed to fully align with water-related SDG targets.

### 3.4. Economic Analysis of the Net-Zero Transition

As shown in Figure 7, MACs exhibit significant uncertainty, especially before carbon neutrality, reflecting deep uncertainty impacts among policy stringency, technology deployment, and demand-side transformation. Cases with stringent cumulative carbon emissions and limited technological progress, which rely heavily on curbing energy service demands, incur significantly higher MACs. Under the CN60 scenario, MACs span 32–527 USD/tCO<sub>2</sub> by 2035, 67–651 USD/tCO<sub>2</sub> by 2060, and 120–222 USD/tCO<sub>2</sub> by 2100. In contrast, MACs will be at least 20% lower than CN60 by 2060 under the CN60E scenario, illustrating the cost-saving synergy of early decarbonization. Moreover, integrating sustainability measures dampens peak MACs under high abatement pressure, indicating that SDG-aligned actions can reduce climate mitigation costs.

The temporal evolution of MACs further reveals a critical reversal in cost dynamics. Prior to carbon neutrality, cases with lower cumulative emissions exhibit higher MACs, reflecting front-load mitigation through demand contraction and early retirement of capital. However, after 2060, this relationship flips. Low-cumulative-emission cases show lower MACs, while high-emission cases face steep costs. This inversion reflects China's transition toward a carbon-negative society, where large-scale CDR deployment becomes necessary. Low-cumulative-emission cases deploy CDR earlier and more gradually, enabling economies of scale and infrastructure reuse that reduce long-term investment. Similarly, while early ambition may entail short-term cost premiums, it unlocks long-term economic and systemic advantages, turning an apparent trade-off into a strategic synergy.

China's net-zero transition is not only a climate imperative but also a powerful engine for high-quality economic growth, driven by massive clean investment and technological innovation. As shown in Figure S18, achieving carbon neutrality requires 7.2–10 trillion USD between 2020 and 2060 (a 24% increase over the REF) and a total of 15–20 trillion USD by 2100 (a 22% increase over the REF). Early action scenario front-loads slightly more capital, requiring 3% additional investment by 2060 (–1.5% to 6%) but reduce long-term outlays, resulting in a 1.8% net increase over the full century.

Solar and wind dominate long-term investment, together accounting for over 65% of energy supply investments. Solar leads marginally, with annual investments averaging 58–100 billion USD compared to 49–83 billion USD for wind. Wind power investment is highly time-sensitive, peaking during 2020–2030 (driven by load growth) and again around 2050 (coinciding with accelerated coal retirements). Meanwhile, energy storage investment rises steadily, reaching 13–25 billion USD annually by midcentury. The CN60 scenario shows the highest investment in wind and solar, underscoring their growing synergy as the backbone of China's postcoal power system.

BECCS, as a critical negative emission technology, sees investment ramp up after 2035 and stabilize at 8.7 billion USD per year after 2060. Crucially, an integrated transformation across the WEF nexus generates significant cost savings. Coordinated policies that reduce water extraction, optimize land use, and moderate bioenergy demand lower the need for BECCS and storage infrastructure, cutting the total system investment by approximately 1%. This demonstrates that

sustainability measures are not only about the environment but also reduce the financial burden of decarbonization.

## 4. DISCUSSION

The study addresses China's dual imperatives of achieving carbon neutrality and advancing long-term sustainable development by integrating energy, land, and water models through a Monte Carlo-based uncertainty framework. By simulating a wide range of plausible futures, we identify the critical uncertainty drivers shaping systematic transformation and technological evolution dynamics across the WEF nexus. Our analysis reveals that net-zero transitions, when aligned with proactive sustainability measures, can catalyze synergistic WEF system transformations. These insights enable the identification of integrated pathways that maximize cobenefits while minimizing potential trade-offs. Our analysis identifies robust policy intervention points that deliver cobenefits across climate and sustainability objectives regardless of future technological or behavioral realizations.

First, an immediate moratorium should be enacted on new coal-fired power plants and accelerate the retrofit or retirement of subcritical units before 2030. Under CN60E, early and decisive action consistently reduces cumulative emissions by 20 GtCO<sub>2</sub>, lowers MACs by 20% by 2060, and avoids 25 Gt per year of additional power sector cooling water post-2035, even under the most pessimistic technology development assumptions.

Second, dietary guidance should be integrated with bioenergy planning. Our results show that scenarios without reduced meat consumption face either food insecurity (below 2700 kcal/cap/day by 2100) or excessive land competition. Conversely, a 15%–20% reduction in animal-based calories by 2035 as sustainability measures modeled in CN60-SDG stabilizes food supply, cuts irrigation water demand by 68 Gt by 2060, and reduces total system investment by 1%.

Third, adaptive carbon budgeting should be institutionalized with transparent rolling targets. Since mitigation ambition is the dominant driver of uncertainty in emission trajectories, China should adopt a legally binding, five-year-reviewed carbon budget framework, starting with a 2035 cap aligned with the cumulative emission reduction identified in the optimized pathways.

Fourth, near-term R&D and demonstration for water-efficient low-carbon technologies should be prioritized. While BECCS is projected to require over 8.7 billion USD per year after 2060, its high water and land intensity risks undermine SDGs. To enhance decarbonization feasibility, targeted subsidies should be directed toward air-cooling retrofits and next-generation infrastructure, ensuring that climate action does not compromise water security.

Fifth, our analysis quantifies a clear trade-off between BECCS expansion and afforestation-based carbon sinks due to competition for land and water. Policymakers should adopt a sequenced carbon removal strategy: prioritize natural climate solutions (such as forest restoration) before 2040, then scale BECCS where sustainable biomass supply and water availability are assured, avoiding uncoordinated deployment that undermines food or ecosystem goals.

Finally, rather than treating climate and sustainability goals separately, we propose to prioritize near-term capital allocation to no-regret, multibenefit interventions. For instance, we recognize that developing wind, PV, and energy storage, as well as exploring nonelectric applications of renewable energy (such

as hydrogen and e-fuels), are critical steps toward balancing sustainability and climate goals.

Overall, the study employed a probabilistic framework to assess more than 4000 uncertainty cases. By quantifying the impact of technological and policy uncertainties, it provides robust evidence to support policymakers in designing synergistic strategies that integrate carbon neutrality targets with the WEF system sustainability. It also offers a reference for other countries seeking to develop coordinated multisystem transformation pathways.

## ■ ASSOCIATED CONTENT

### SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.est.6c03030>.

Model interconnection framework diagram; CO<sub>2</sub> captured by CCUS; demand change for different energy service demand; the correlation between input uncertain variables and key output variables; daily calorie intake per capita and calorie share of animal-sourced foods; water supply and withdrawal; cooling type of thermal power; investment demand for the China's net-zero transition; energy and climate policy list; sustainability measures list; technoeconomic parameter assumptions; parameter probability distribution assumptions; and China TIMES 2.0 model introduction (PDF)

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S.Z.: writing—original draft, visualization, software, resources, methodology, investigation, formal analysis, data curation, conceptualization, funding acquisition. W.C.: writing—review and editing, supervision, project administration, funding acquisition.

### Notes

The authors declare no competing financial interest.

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