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Assessing uncertain technological progress in the decarbonization pathway of China's hydrogen energy system

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ABSTRACT

Hydrogen energy is regarded as a promising solution for decarbonizing hard-to-abate sectors, while its role in the energy transition remains debatable. One of the key reasons is that uncertainty in technological progress has significant impacts on investment decision-making. To assess these effects, this study employs the MESSAGEix framework to develop a hydrogen energy system optimization model in China's context and integrates it with a stochastic scenario-tree generation method to assess the effects of uncertain technological progress on decarbonizing China's hydrogen energy system. The modeled system covers a full range of hydrogen production and consumption associated with different technical options for decarbonization, i.e., renewable energy-based water electrolysis (green hydrogen) and fossil-derived hydrogen coupled with carbon capture and storage. The model simulates a wide range of stochastic crucial cost metrics under the carbon-neutral constraint and compares it to a baseline without an emission constraint. Results show that disruptive technological breakthroughs in renewable electricity generation are essential to decarbonizing the hydrogen production system. The proposed hybrid modeling approach proves that computing is effective and could be applied to many other stochastic programming problems in long-term energy system planning.

1. Introduction

Green hydrogen, i.e., using surplus renewable electricity to produce hydrogen through water electrolysis, emerged as a promising solution to address the mitigation challenge in the 'hard-to-abate' (HTA) sectors (Yang et al., 2022). Hydrogen energy has been experiencing hot debates globally, and many pilot projects are now being developed worldwide (Chehade et al., 2019; Megy and Massol, 2023).

China is the world's largest producer and consumer of hydrogen, with an annual output of about 35 million tons (Mton), accounting for one-third of global demand (Department of Science and Technology, National Energy Administration, 2024). Hydrogen has been widely used in the chemical industry, refineries, and transportation sectors in China. On the supply side, China's hydrogen production is dominated by the coal-based technological route and has a high carbon intensity. The Chinese government attaches great importance to the development of the hydrogen industry and released the 'Medium and Long-Term Plan for the Development of the Hydrogen Energy Industry (2021-2035)' in 2022. This plan clarifies the strategic positioning of hydrogen in China's future energy structure and sets development goals for different stages. For the first time, it systematically proposes large-scale applications of hydrogen beyond the transportation sector, including energy storage, power generation, and industrial uses, pointing the way for the development of the hydrogen industry.

It is important to note that technological progress in developing a green hydrogen economy faces substantial uncertainties. It remains unclear when and how fast the low-carbon technologies in the hydrogen supply chain, including renewable electricity generation, water electrolysis, and carbon capture and storage (CCS) would become cost-competitive. This lack of knowledge becomes a challenge in the decision-making of a low-carbon transition pathway of the hydrogen energy system that may incur enormous risks of sunk investments. Some latest studies explore the potential of green hydrogen in realizing a decarbonization target in the middle to long run (Li et al., 2021; Oshiro and Fujimori, 2022; Yang et al., 2022). Nevertheless, a comprehensive assessment of the effects of uncertain technological progress on

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decarbonizing China's hydrogen energy system is insufficient.

This study attempts to address this challenge by developing a hybrid modeling framework that integrates stochastic scenario-tree generation with a long-term hydrogen energy system planning model to assess the effects of uncertain technological progress on the hydrogen decarbonization pathways. To this end, we first construct a multi-period long-term energy system optimization model with rich technological information to explore the least-cost pathways of China's hydrogen system transition. Second, we develop a scenario tree method able to generate a wide range of possible techno-economic metrics of the key technologies to reflect the uncertainties in technological advancement. This hybrid modeling framework enables computing a large set of scenarios categorized into two ensembles, i.e. a baseline and a carbon neutral, and to simulate and compare the system performances and the effects of uncertain technological progress in the two settings. To our knowledge, this is the first study of its kind to attempt to address the energy system optimization problem facing uncertain technological progress in modeling hydrogen energy system transition.

The paper is structured as follows. After this introduction, Section 2 summarizes the latest research in energy system planning models and methods employed for dealing with uncertainty in these models. Section 3 describes in detail the modeling framework, including the construction of China's hydrogen energy system model, the stochastic scenario tree generation method, the simulation method of multiple cost variables, and how different components are integrated. Section 4 introduces the data and parameters, as well as the scenario settings. Section 5 presents the analysis of the scenario results, in particular the implications on CO_2 emissions pathways, production mixes, and investment. The final Section 6 concludes and discusses the policy implications.

2. Literature review

2.1. Modeling hydrogen energy system

Studies on the integrated modeling of hydrogen energy system are still rare but have been increasing in recent years. Earlier work includes assessment of the role of hydrogen in country-level energy transition, e.g. Bae and Cho (2010) analyze the dynamic economic impacts of building a hydrogen economy in Korea employing a dynamic Computable General Equilibrium (CGE) model.

A few more recent examples have extended the model development and research frontiers in several aspects. Bucksteeg et al. (2023) extend a detailed bottom-up market model by including the PtG technology and competing flexibilities. Several scenarios are developed regarding levels of CO_2 price, techno-economic parameters of flexibilities and shares of variable renewable energy sources for 2025. vom Scheidt et al. (2022) link an electrolytic hydrogen supply chain model with an electricity system dispatch model and perform a cross-sectoral case study of Germany in 2030, and find that hydrogen infrastructure investments and their effects on the electricity system are strongly influenced by electricity prices. Yang et al. (2022) improve the China-MAPLE model which is based on the TIMES (The Integrated MARKAL-EFOM System) modeling framework by in-depth representation of hydrogen energy production and consumption sectors in China's energy system, and use the model to evaluate the prospective role for clean hydrogen in the HTA sectors in China.

Despite these efforts exert enormous impacts on the development pathways of hydrogen energy system and the associated CO2 emissions, the uncertainties of the technology progress in the hydrogen supply chain. It is, however, also widely acknowledged that these factors determine the relative advantage of hydrogen versus other energy carriers, and a lack of representation in hydrogen-related ESMs may lead to sub-optimal design decisions in energy policy-making.

2.2. Energy system planning with uncertain factors

Strategic energy system planning often deals with the capacity expansion of energy installations or infrastructure in the long-term transition. Uncertain information is prevalent in the process of energy system planning; incorporating uncertain factors is of great importance since ESMs usually require inputs of a variety of different technical and economic parameters difficult to determine in the long-term modeling horizon, such as technology investment costs, energy prices, technology efficiency, and carbon price (Huppmann et al., 2019). Moreover, these models are generally large-scale and represent a large number of technologies covering the whole energy system from primary energy supply to final energy consumption. Ma (2010) models uncertain endogenous technological change in a stylized model to illustrate the evolution of a few representative technologies. Whereas the non-linearity caused by the endogenous technological change is computationally prohibitive in the full-fledged energy system model that may have hundreds of technologies.

Various methods could be used in combination with ESMs to reflect uncertainties in energy systems planning. Sensitivity analysis, for example, is a crucial method for assessing the robustness of model outputs to variations in key input parameters. Sensitivity analysis identifies the most influential factors affecting model outcomes by systematically altering inputs like fuel prices, technology costs, demand growth, or policy constraints. This approach helps to understand the uncertainty and potential variability in energy system projections, guiding policymakers in making informed decisions. Sensitivity analysis also aids in identifying critical areas where more precise data or assumptions are needed, ensuring that the model results are reliable and reflect possible real-world scenarios.

Unlike sensitivity analysis used for targeted analysis, which provides insights into how specific assumptions impact model results, Monte Carlo simulations involve randomly sampling input parameters from predefined probability distributions and running the model numerous times to generate a range of possible outcomes. It captures the full spectrum of potential uncertainties and provides a probabilistic distribution of outcomes, offering a more comprehensive view of risk and uncertainty. For example, Zhang and Chen (2022) developed a Monte Carlo analysis method in an energy-environment-economy model to generate 3000 cases of different technological evolution pathways and carbon peak time. This study demonstrates the application of the Monte Carlo method in large-scale ESMs. It should be noted that the Monte Carlo approach has deficiencies in the simulation of multi-variate time series data (Yue et al., 2018), and thus cannot characterize trends in parameters over time. To overcome this shortcoming, time-series technology-based approaches were employed in some studies. For instance, autoregressive integrated moving average with exogenous variables (ARIMAX), Ornstein-Uhlenbeck process, and a geometric Brownian motion were constructed for modeling uncertainties of the energy price and carbon price in an energy system optimization model (Ren et al., 2021). The data-driven and machine-learning approach represents another paradigm that requires detailed historical data (Jain et al., 2017). However, these uncertainty analysis methods usually have the disadvantage of being computationally inefficient when the complexity of the problem increases. Furthermore, these methods cannot handle the parameter without historical data or probability distributions (Høyland and Wallace, 2001).

Scenario tree generation represents another method used to represent various future pathways in a structured and hierarchical manner in energy systems modeling (Kim et al., 2019; Oliveira et al., 2015). This approach is beneficial in dealing with uncertainties over time, such as changes in technology, policy, demand, or resource availability.

2.3. Selection of MESSAGEix and scenario tree

The MESSAGEix modeling framework is an advanced, integrated assessment tool designed for analyzing energy systems, environmental impacts, and economic policies. Developed by the International Institute for Applied Systems Analysis (IIASA), it enables the exploration of future scenarios by linking energy production, consumption, and associated emissions with economic and policy decisions (IIASA ECE Programme, 2020). MESSAGEix supports long-term planning by optimizing energy systems under various constraints, considering technological development, resource availability, and policy measures. It is highly flexible, allowing customization for specific regions or sectors, and is widely used for climate change mitigation, sustainable development, and energy transition studies (Krey et al., 2020; Zakeri et al., 2022). MESSAGEix is open-source and easily connects with other uncertainty analytic methods.

Scenario tree generation is used in long-term energy planning, climate change mitigation strategies, and investment decisions in energy systems. It provides a systematic way to explore and manage uncertainty, making it a valuable tool for policymakers and planners. In this approach, scenarios can be assigned probabilities to reflect the likelihood of different outcomes, helping to weigh the impact of decisions under uncertainty. This allows for a probabilistic assessment of risks and opportunities. It provides a systematic way to explore and manage uncertainty, making it a valuable tool for policymakers and planners. Studies have used scenario trees based on qualitative or quantitative methods to model uncertain parameters, for example, using the moment matching method to generate an appropriate scenario tree for the photovoltaic module price (Kim et al., 2019), and using the conditional generative adversarial network–random forest–Markov chain (CGAN–RF–MC) method to generate a scenario tree of multi-energy load profiles (Lei et al., 2021).

As summarized above, modeling uncertainty is of great importance in energy system planning to capture future parameters' evolution, especially in a long-term modeling horizon. We are unaware of studies on the integrated modeling of hydrogen with energy optimization models that have considered the uncertainty of hydrogen technology (e.g., how the costs of hydrogen technology will evolve in the future). This study attempts to fill this gap by incorporating the uncertainty of hydrogen technology advancement in an integrated energy system model built on MESSAGEix to investigate how the uncertainty of hydrogen technology will affect the hydrogen production mix, emission pathways, and optimal investments.

3. The modeling framework

3.1. Description of the modeled hydrogen energy system

The modeled hydrogen energy system is illustrated in Fig. 1, where different colored shapes represent different components in the system. The yellow indicates conventional fossil fuel-based technologies, mainly including the coal gasification route and the SMR route, which uses natural gas as the feedstock. The green shapes represent the more innovative technologies, i.e., those in the green hydrogen supply chain. This supply chain mainly consists of renewable electricity generation such as solar PV and wind farms, as well as water electrolysis that splits water into the main product, hydrogen, and the byproduct, oxygen. Furthermore, electricity storage, such as batteries, is also required for stable production conditions. Besides the renewable electricity-based green hydrogen production, another electrolysis route using grid electricity has a declining carbon footprint from 25 to 4 $kgCO_2/H_2$. It is noteworthy that water electrolysis with renewable electricity is not the only way to cut the CO_2 emissions of hydrogen production. Another approach is to install carbon capture and storage (CCS) to the existing conventional capacities. Hydrogen produced from this route is also

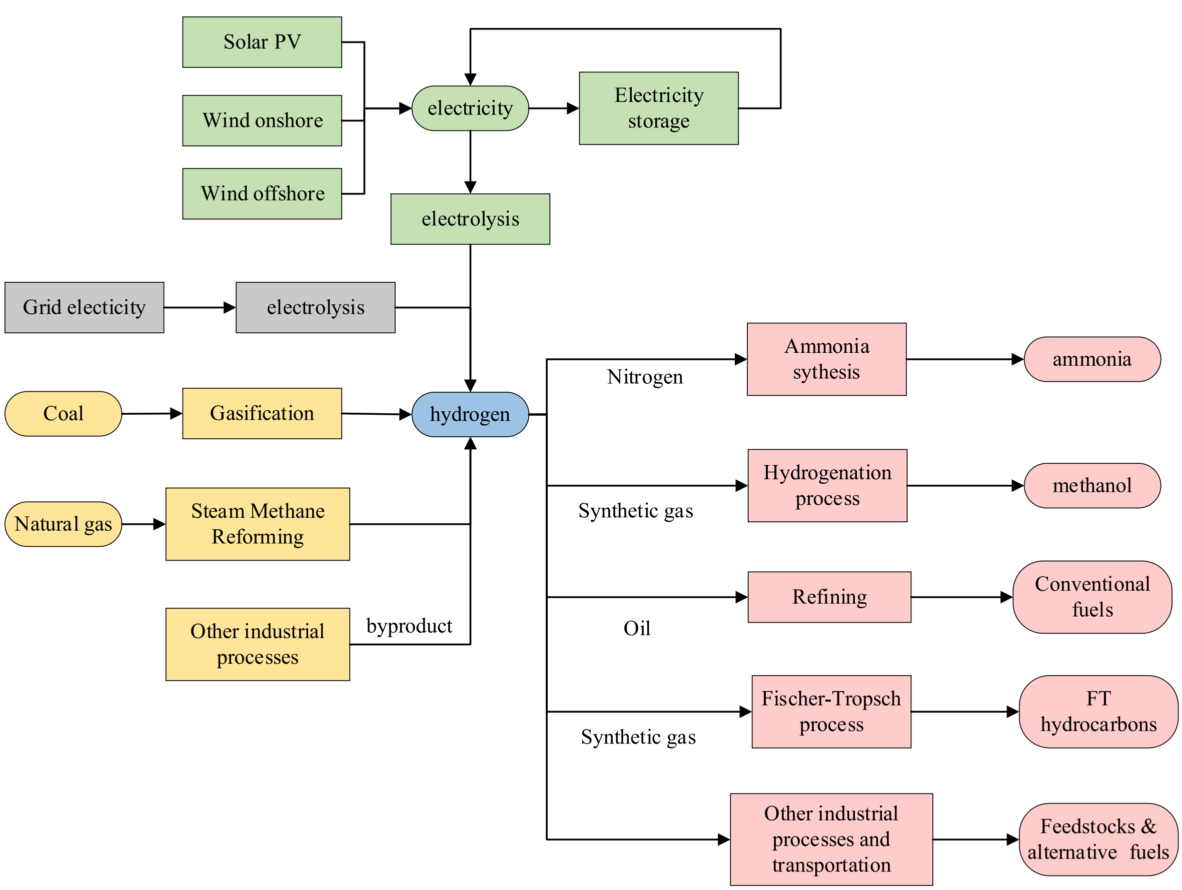

Fig. 1. The hydrogen energy system modeled in this study.

called 'blue hydrogen'.

The typical downstream products using hydrogen as feedstock include ammonia, methanol, refinery fuels, Fischer-Tropsch (FT) fuels, other industrial processes, and transportation fuels such as fuel cell vehicles.

3.2. The linear optimization model

As described above, we consider different technologies for hydrogen production: $\mathscr{T}^{H_2} = \left\{H_2^{coal}, H_2^{gas}, H_2^{byp}, H_2^{elec}\right\}$, Coal gasification ($H_2^{coal}$), steam methane reform (H_2^{gas}), and hydrogen embedded in byproducts from industrial processes (H_2^{byp}) are well-established and have a long history of development and application. In light of this, these conventional fossil fuel technologies are assumed with no further advancements in the future. The electricity-based hydrogen production (H_2^{elec}) has three technological options. The alkaline route ($H_2^{elec,alk}$) is matured and has been widely adopted in some industrial processes. PEM ($H_2^{elec,pem}$) and SOEC ($H_2^{elec,soec}$), representing the future direction, are more advanced and efficient but at an early stage of development. The two advanced technologies have higher capital costs compared to the alkaline process. Nevertheless, substantial cost decreases of these two technologies could be anticipated as intensive R&D activities are put in these areas worldwide. The upstream electricity could come from three renewable power generation technologies: $\mathscr{T}^R = \{solar, wind\ onshore, wind\ offshore\}$.

This system design enables zero-emissions hydrogen production. Note that all three renewable technologies produce intermittent electricity and add volatility to the electricity system. A complete simulation of a high-share renewable energy system necessitates a dedicated electricity dispatch model. Nevertheless, incorporating such an electricity dispatch model into calculating a large set of scenarios with uncertainty would be computing prohibitive and would also shift the research focus of this study. Following the approach introduced by (Sullivan et al., 2013), we employ a reduced-form, dynamic, accounting of reliability and variability in MESSAGEix, that is, introducing electricity storage as a balancing technology governing load-following and ancillary services to meet the requirement without adding substantially to the complexity of the model.

There are a variety of commodities $m \in \mathscr{M}$ in the modeled hydrogen energy system, in which hydrogen serves as the core intermediate energy carrier. In different production processes, crucial energy commodities for hydrogen production include: $\mathscr{M}^e = \{hydrogen, electricity, coal, oil, gas\}$. Some other commodities, such as water for hydrogen production and nitrogen for ammonia production, are also included in the modeled system. These non-energy commodities are assumed to be sufficient with no scarcity to keep the research focused. As a result, volumes of these commodity supplies have no impact on the model results. The system operates at the minimum cost to meet the exogenous demands of five final products that use hydrogen as the feedstock: $M^p = \{ammonia, methanol, oilfuels, chemicals, heat, transport\}$.

- Sets

$m \in M$, commodity in the hydrogen energy system.

$p \in P$, final product in the hydrogen energy system, $P \subset M$.

$t \in T$, technology in the hydrogen energy system.

$t' \in T^{L'}$, technology at the downstream level L' that uses commodity m as the feedstock (or input). $T^{L'} \subset T$.

$y \in Y$, index of modeling year, $Y = Y^M \cup Y^H$, Y^M is the set of modeling years, $Y^M = \{2025, 2030, \dots, 2060\}$, and Y^H is the set of historical years, $Y^H = \{2000, 2005, \dots, 2020\}$.

y^s, y^e, the first and last modeling year, respectively.

y^i, installation year of technology t, $y^i \in Y$, $y^i \leq y$

- Parameters

dr, discount rate.

τ, time interval.

$c_{t,y}^{inv}$, unit investment cost for technology t in year y, Myuan/unit capacity.

$c_{t,y^i,y}^{fo}$, unit fixed operations and maintenance (O&M) cost in year y for the capacity of technology t installed in year y^i, Myuan/unit capacity.

$c_{t,y^i,y}^{vo}$, unit variable cost in year y for the capacity of technology t installed in year y^i, Myuan/unit output.

$pr_{m,y}$, price of commodity m in year y, yuan/ton or yuan/MWh.

lf_t, lifetime of technology t, years.

$\eta_{m,t}^{in}$, coefficient of converting feedstock commodity m to other commodities by technology t.

$\beta_{c,t}$, capacity factor of the existing capacity of technology t.

λ_t, CO_2 emission factor of technology t. tonCO_2/unit output.

- Decision variables

$NC_{t,y}$, decision variable for newly added capacity of technology t in year y.

$EC_{t,y^i,y}$, existing capacity of technology t in year y for capacity installed in year y^i

$HC_{t,y}$, auxiliary variable, historical installed capacity of technology t in year y, Mton/yr.

$OP_{m,t,y^i,y}$, output of technology t in year y for capacity installed in year y^i using commodity m as the feedstock

$EM_{t,y}$, CO_2 emissions of technology t in year y, Mton/yr.

The model is constructed according to the relationship and constraints of the following equation. The objective function is to minimize the total cost (TC) of all technologies in the hydrogen supply chain over the modeling horizon from 2025 until 2060, as shown in Eq. (1). The total cost mainly comprises four components, the capital investment costs for newly added capacities $c_{t,y}^{inv} \cdot NC_{t,y}$, the fixed O&M costs for the existed operating capacities $c_{t,y^i,y}^{fo} \cdot EC_{t,y^i,y}$, the variable O&M costs related to the output of commodity m $c_{t,y^i,y}^{vo} \cdot OP_{m,t,y^i,y}$, and the procurement of upstream feedstocks $pr_{m,y} \cdot \eta_{m,t}^{in} \cdot OP_{m,t,y^i,y}$. Note that $\eta_{m,t}^{in} \cdot OP_{m,t,y^i,y}$ represents the feedstock input required for producing unit product m by technology t.

Let y^s and y^e represent the start and end modeling year, respectively, and the time interval τ be five years. Therefore, the model optimizes over all the years $y \in Y^M = \{2025, 2030 \dots, 2060\}$. To represent currently existing capacities that were installed in historical years, a set of historical years $Y^H = \{2000, 2005, \dots, 2020\}$ is also defined, and another year index y^i is added to track the installation time of different capacity cohorts for the same technology. This index then falls into the full set of the whole timespan $y^i \in Y = Y^M \cup Y^H$ and is subject to the constraint $y^i \leq y$. All the costs occurring in year y are discounted to the present value of the starting year y^s.

$$\begin{aligned} min \quad TC = & \sum_t \sum_y c_{t,y}^{inv} \cdot NC_{t,y} \Big/ (1+dr)^{(y-y^s)} \\ & + \sum_{(t,y^i,y)} c_{t,y^i,y}^{fo} \cdot EC_{t,y^i,y} \Big/ (1+dr)^{(y-y^s)} \\ & + \sum_{(t,y^i,y)} \sum_m c_{t,y^i,y}^{vo} \cdot OP_{m,t,y^i,y} \Big/ (1+dr)^{(y-y^s)} \\ & + \sum_{(t,y^i,y)} \sum_m pr_{m,y} \cdot \eta_{m,t}^{in} \cdot OP_{m,t,y^i,y} \Big/ (1+dr)^{(y-y^s)} \end{aligned} \tag{1}$$

The relation between existing capacity $EC_{t,y^i,y}$ and newly added capacity $NC_{t,y}$is expressed by Eq. (2), where an auxiliary variable $HC_{t,y}$ is added for tracking historical installations. Note that this relation conforms to the constraint $y - y^i \le lf_t$. This constraint ensures that capacities with an age longer than the lifetime lf_twould be retired from existing capacities at year y

$$\sum_{y^i} EC_{t,y^i,y} = HC_{t,y} + NC_{t,y} \forall t \in T, y \in Y^M, y - y^i \le lf_t \tag{2}$$

At the final level of the supply system, demand for each final product $p \in \mathscr{P}$ should be always met by the corresponding production technology t^p, as shown in Eq. (3):

$$\sum_{(t,y^i,y)} OP_{p,t,y^i,y} \ge dmd_{p,y} \quad \forall p \in P, \ (t,y^i,y) \in TYY^M \tag{3}$$

For each level L in the supply chain, energy balances are ensured by Eq. (4):

$$\sum_{(t,y^i,y)} OP_{m,t,y^i,y} = \sum_{(t',y^i,y)} \eta^{in}_{m,t'} \cdot OP_{t',y^i,y} \quad \forall m \in M, (t,y^i,y) \in TYY^M \tag{4}$$

The production processes also conform to capacity constraints expressed by multiplying the existing capacity of technology t with the corresponding capacity factor $\beta_{c,t}$, as shown in Eq. (5):

$$OP_{m,t,y^i,y} \le EC_{t,y^i,y} \cdot \beta_{c,t} \quad \forall m \in M, \ (t,y^i,y) \in YY^M \tag{5}$$

CO_2 emissions of technology t, $EM_{t,y}$, are calculated by multiplying the output with the corresponding carbon emission rate λ_t, and summing over all the capacities.

$$EM_{t,y} = \sum_{(t,y^i,y)} \sum_m OP_{m,t,y^i,y} \cdot \lambda_t \quad \forall t \in T, \ y \in Y^M \tag{6}$$

3.3. Modeling uncertain technological advancement

As described in Section 3.1, the whole hydrogen energy system consists of several levels of technology chains. At each level, several competing technologies vary in capital cost, energy efficiency, and other techno-economic metrics. These technologies are at different stages of development, as such they differ in potential for further advancement in the future.

To quantify the impacts of uncertain technology advancement, we assume that over the modeled horizon, the cost parameters $c^{inv}_{t,y}$, $c^{fo}_{t,y^i,y}$ and $c^{vo}_{t,y^i,y}$ decline for innovative technologies, and remain stable for matured technologies. Two technology sets, $T^{H_2^{elec}}$ and T^R, representing hydrogen production from electrolysis and renewable electricity generation, respectively, are considered to have the potential of cost reduction with different declining rates. Hereafter we use $T^N = T^{H_2^{elec}} \cup T^R$ to denote the set of these new technologies with varying cost parameters, while for those technologies not in this set $t \notin T^N$, the cost parameters are assumed constant over the modeling horizon. We use geometric Brownian motion (GBM) to model the varying cost metrics (denoted as a generalized variable $c_{t,y}$for both investment costs and O&M costs), and express their forms in stochastic differential equation (SDE) shown as Eq. (7):

$$\frac{dc_{t,y}}{c_{t,y}} = \mu_t dy + \sigma_t dW_{t,y} \quad \forall t \in T^N, y \in Y^M \tag{7}$$

where μ_t and σ_t represent the percentage drift and the percentage volatility, respectively, and $W_{t,y}$ is a Brownian motion. The analytic solution of the SDE could be employed for simulating the values of cost parameters of technology t at every instant of temporal discretization, expressed by Eq. (8):

$$c_{t,y+\tau} = c_{t,y} \cdot e^{\left(\mu_t - \sigma_t^2/2\right)\tau + \sigma_t \sqrt{\tau} W_{t,n+1}} \quad \forall t \in T^N, y \in T^M \tag{8}$$

As described in Section 3.1, The hydrogen energy system model takes in various cost parameters of many technologies simultaneously. Hence a multi-dimensional geometric Brownian motion is employed for scenario tree generation. Here we define a covariance matrix $\Sigma_{t^i,t^j} := \rho_{t^i,t^j} \sigma_{t^i} \sigma_{t^j}$, where t^i and t^jrepresent cost parameters for the i^{th} and j^{th} technology in the set T^N, respectively, and ρ_{t^i,t^j} is the correlation coefficient of the Brownian motion terms W_{t^i} and W_{t^j} in Eq. (8), i.e., $\rho_{t^i,t^j} = corr[W_{t^i}, W_{t^j}]$. The covariance of $c_{t^i,y}$and $c_{t^j,y}$ is given by Eq. (9).

$$Cov\left[c_{t^i,y}, c_{t^j,y}\right] = c_{t^i,y^s} \cdot c_{t^j,y^s} \cdot e^{\left(\mu_{t^i} + \mu_{t^j}\right)\frac{y-y^s}{\tau}} \left(e^{\rho_{t^i,t^j} \sigma_{t^i} \sigma_{t^j} \frac{y-y^s}{\tau}} - 1\right) \tag{9}$$

The covariance matrix Σ_{t^i,t^j} could be decomposed into $\Sigma_{t^i,t^j} = AA^T$ where A is a matrix that allows $AW_{t^i,y}$ to represent a GBM process without drift (Glasserman, 2004). By incorporating this property, the GBM for a single cost metric could be transformed and employed for simulating the multi-dimensional GBM process, as shown in Eqs. (10) and (11):

$$\frac{dc_{t^i,y}}{c_{t^i,y}} = \mu_{t^i} dy + \sum_{t^j \in T^N} A_{t^i,t^j} dW_{t^j,y} \tag{10}$$

$$c_{t^i,y+\tau} = c_{t^i,y} \cdot e^{\left(\left(\mu_{t^i} - \sigma_{t^i}^2 / 2\right)\tau + \sum_{j \in T^N} A_{t^i,t^j} \sqrt{\tau} W_{t^j,y+\tau}\right)} \quad \forall t \in T^N, y \in Y^M \tag{11}$$

3.4. Scenario tree generation

The scenario tree method has been widely used in models of decision-making under uncertainty. Differing from other uncertainty analysis methods, such as sensitivity analysis, scenario tree generation is better suited for stochastic optimization to represent uncertainties over time. It involves creating a tree structure where each branch corresponds to a possible realization of uncertain parameters at different stages with associated probabilities. This method captures the evolution of uncertainty and allows the model to optimize robust decisions across multiple future scenarios.

In the hydrogen model, one scenario represents realizations of all random variables, i.e., the cost metrics for $t \in T^N$, in all modeled years. We follow the procedure proposed by Høyland and Wallace to generate scenarios for the hydrogen energy system optimization model (Høyland and Wallace, 2001). This scenario tree generation method is based on a nonlinear optimization programming to minimize some measures of distance between the statistical properties of the generated outcomes and the specified properties (Høyland and Wallace, 2001). Fig. 2 illustrates scenario three of the model that branches off for each possible value of the cost metric $c'_t = \left(c_{t,y^s}, c_{t,y^s+\tau}, \dots, c_{t,y^e}\right)$ at each stage $y = y^s, \dots, y^e$.

This optimization-based multivariate scenario tree-generating method can also be referred to as moment matching. As shown in Fig. 2, each child node that contains multivariate in the cost metric vector $\boldsymbol{c_t}$ is generated from the conditional distribution of its parent node. For example, nodes at $y = y^s + \tau$ are generated from the conditional distribution at $y = y^s + \tau$with respect to the node at $y = y^s$, and the upper two nodes at $y = y^s + 2\tau$ are generated from the conditional distribution with respect to the first node $y = y^s + \tau$. Let N be the node set that contains the subset N_y at each modeling stage $y \in Y^M$. Let S be the set of all specified statistical properties, S^{val}_sbe the specific value of a statistical property $s \in S$, and p_n be the probability of node $\boldsymbol{n}$. The mathematical expression for statistical property s is $f_s(c_t, p)$. The nonlinear optimization model is to minimize the weighted square sum of differences between the values of statistical measures from the estimated GBM process, subject to constraints defining the nonnegative probabilities to sum up to one and to be within the range of an upper bound ub^p, as shown by Eqs. (12)–(14).

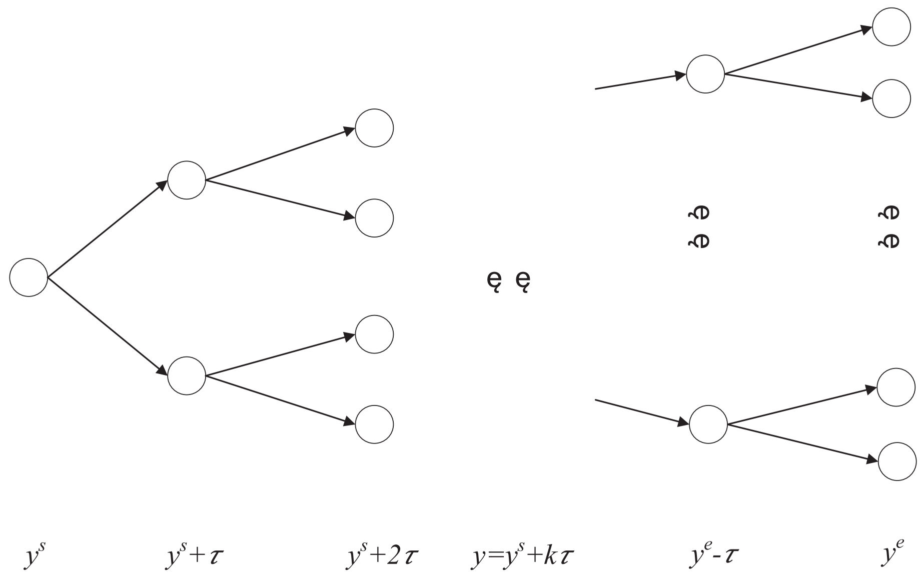

Fig. 2. The scenario tree of the cost metrics.

$$\min_{c_t,p} \sum_{s\in S} w_s \cdot \left(f_s(c_t,p) - S_s^{val}\right)^2 \quad \forall y \in Y^M \tag{12}$$

$$s.t. \quad \sum_{n\in N_y} p_n = 1 \tag{13}$$

$$0 \le p_n \le ub^p, \quad \forall n \in N \tag{14}$$

In this study, mean, standard deviation, skewness and kurtosis are used as the statistical measures, and all weights w_s are set to 1.

4. Data and assumptions

4.1. Data for technological economics and performance

We have compiled data for model parameterization, including costs, conversion efficiency, lifetime, existing capacities, and economic parameters and assumptions. Tables 1 and 2 present key techno-economic parameters and assumptions for the technologies in the set $\mathscr{T}^N$ that are considered with a higher potential for cost reduction in the future. For the sake of brevity, other important parameters and assumptions in the model are provided in the Supplementary Information (SI). Note that the cost parameters in the tables represent the current techno-economics at the starting year y^s, i.e., the initial values for the GBM processes specified in Section 3.2. For CCS-related technologies, it is assumed that the addon part of CCS will have cost reduction potential, whereas the cost for the component of conventional fossil fuel-based process is assumed constant. For instance, the cost of coal gasification with CCS consists of a constant cost component of coal gasification and a declining component of CCS. As a result, the overall cost of coal gasification with CCS will have a moderate declining trend that will remain above the cost of the cost without CCS.

4.2. Parameters for simulating uncertain technological advancement

The key parameters used in the GBM processes to simulate cost variations with uncertain technological advancement are summarized in Table 3. The parameters are obtained in the following approach. First, we collect the data of current techno-economics for the technologies in $\mathscr{T}^N$ (as summarized in Tables 1, 2, and in the SI), which are used as the initial values for the starting year y^s in the GBM processes. We then categorize these technologies according to their current technology readiness level (TRL) and compile the cost data for the end year y^e mainly through expert elicitation. These expert-elicited data vary in certain ranges and are subject to different levels of uncertainty. For a single technology, the average cost is used as the value for y^e in the deterministic GBM process with the volatility parameter σ_t equal to zero. Knowing the values for y^s and y^e, we then estimate the drift parameter μ_t in the GBM process that dictates the downward slope of the cost declining trend. Subsequently, we use the range of expert-elicited data to estimate the parameter σ_t in the stochastic processes. The simulation results of the investment cost declining paths using the GBM processes

Table 1
Key techno-economic parameters for fossil fuel hydrogen production, renewable electricity generation, and storage technologies.

	CAPEX (RMB/kWe)	OPEX (RMB/kWe)	Efficiency	Lifetime (years)
Coal gasification	24,800 RMB/ tH_2/a	1240 RMB/ tH_2/a	60 %	25
Coal gasification with CCS	34,335 RMB/ tH_2/a	1717 RMB/ tH_2/a	58 %	25
SMR	10,600 RMB/ tH_2/a	265 RMB/ tH_2/a	76 %	25
SMR with CCS	16,860 RMB/ tH_2/a	520 RMB/ tH_2/a	69 %	25
Methanation	3850 RMB/ tProd/a	155 RMB/ tProd/a	77 %	30
Fischer-Tropsch	4050 RMB/ tProd/a	162 RMB/ tProd/a	73 %	30
Solar PV	4100 RMB/ kWe	78 RMB/ kWe	12 %	25
Wind onshore	6700 RMB/ kWe	320 RMB/ kWe	21.5 %	25
Wind offshore	16,500 RMB/ kWe	650 RMB/ kWe	25 %	25
Electricity storage	1250 RMB/ kWe	10 RMB/ kWe	95 %	10

Table 2
Key techno-economic parameters for three P2G technologies.

	CAPEX (RMB/ kWe)	OPEX (RMB/ kWe)	Efficiency	Stack lifetime (hours)
Alkaline	3250	1.5 %	66 %	75,000
PEM	7150	1.5 %	58 %	50,000
SOEC	18,200	1.5 %	77 %	20,000

Table 3
Parameters in the GBM processes for simulating cost variations.

	Solar PV	Wind onshore	Wind offshore	Electricity storage	H2-alkaline
μ_t	−0.016	−0.021	−0.023	−0.028	−0.012
σ_t	0.015	0.018	0.019	0.023	0.014
	H2-PEM	H2_SOEC	H2-coal-CCS	H2-SMR-CCS	
μ_t	−0.028	−0.04	−0.015	−0.015	
σ_t	0.025	0.032	0.014	0.014	

are presented in Fig. 3.

The simulation results show that uncertainty in technological progress varies across different technologies despite a general downward trend for all the technologies. For some technologies at their earlier R&D stage, such as electricity storage, PEM, and SOEC for electrolysis, are with lower TRL and would have larger potentials for cost reduction as intensive R&D activities are put in these areas. Renewable energies including solar PV and wind farms have achieved commercialization for many years and have been widely installed nowadays. These technologies with higher TRL are still in progress, but their cost reduction potentials are relatively smaller.

4.3. The carbon neutral scenario

China has set ambitious 'dual carbon goals' (also known as the 2030/2060 goals), described as reaching its carbon emissions peak in 2030 and becoming carbon neutral before 2060. In line with these goals, this study sets a carbon-neutral scenario to peak the total emissions from the whole hydrogen energy system by 2030 and become net-zero by 2060. Eq. (15) expresses the constraints of total emissions added to the model in this scenario. The constraint requires that the annual CO_2 emissions from the system, expressed by the term $\sum_t EM_{t,y}$ that adds up all the emissions from each technology, should not exceed an emission bound emb_y.

$$\sum_t EM_{t,y} \le emb_y \quad \forall t \in T, \ \ y \in Y^M \tag{15}$$

It is noteworthy that there might be a small portion of emissions from some HTA sectors with extremely high abatement costs. This part of residual emissions could be offset by carbon removal technologies such as biomass with carbon capture and storage (BECCS). Studies on the national carbon-neutral pathways show that the residual emissions in 2060 range from 2 to 8 % of the base year (He et al., 2021, 2022; Yu et al., 2023; Zhang and Chen, 2022). Accordingly, we set the CO_2 emissions bound in 2060 as 5 % of the emissions in 2020, indicating deep decarbonization of the energy system. These emission constraints added in the carbon-neutral scenario could be interpreted as some potential regulatory policies or emissions trading schemes (ETS) that aim to control the total amount of emissions from a region or an industry. For instance, ETS puts a limit on the total emissions from the whole industry and allocates emissions quota amongst firms, but allows for flexible market trading of these quotas. It has been widely implemented in many countries.

The carbon neutral scenarios are set and simulated to compare with the baseline scenarios which are assumed with no emission constraints. Both two sets of scenarios are subject to uncertain progress of the selected innovative technologies, the cost parameters of which are shown in Fig. 3.

5. Scenario results and analysis

5.1. Emissions pathways

The pathways of the total CO_2 emissions from the entire hydrogen energy system are presented in Fig. 4. The yellow and blue lines represent the deterministic cases for the baseline and the carbon neutral

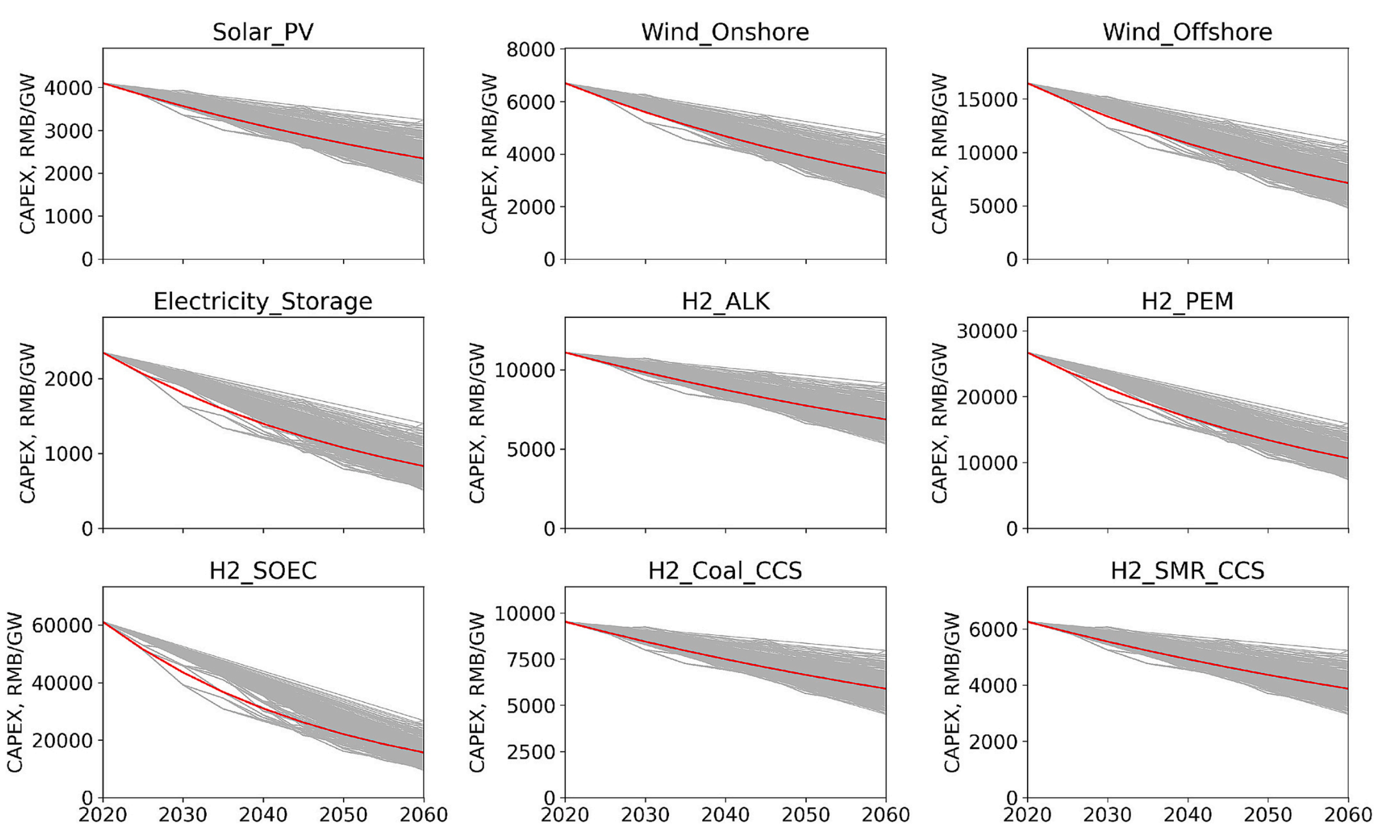

Fig. 3. The simulated paths of investment costs with uncertain technological progress. Note: the red line in each panel represents the deterministic case for each technology. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

scenario respectively. The shaded areas indicate uncertain ranges of the two scenario ensembles. It is noteworthy that this study assumes demands are changing in a deterministic pattern; that is, the demand for a single final product is assumed to be the same for all the scenarios, where only techno-economic parameters are subject to uncertainty. Only with this assumption are the scenarios comparable concerning techno-economics and carbon constraint uncertainties. As a result, the emissions pathways overlap before 2030 because most of the existing installations remain operational to meet the demands of the final products. The whole energy system gradually evolves as new capacities are installed and older existing capacities are phasing down, leading to completely different technology mixes and emissions profiles.

The baseline with no emission constraints shows a wide range of emission pathways with uncertain technology advancement. In the deterministic case, the total CO_2 emissions will not peak until the horizon's end. These emissions increase from 366 Mton in 2020 to 499 Mton in 2035, then jump to 675 Mton in 2045. The period between 2035 and 2045 sees rapid growth because, without the carbon emissions constraint, the cheap coal-based route is opted for after the retirement of existing capacities. Whereas as the cost of renewable-based hydrogen drops to a level with competitiveness, more green hydrogen capacities are installed, and the rising trend of emissions is curbed after 2045. However, this is not always the case for other scenarios. The extreme scenario with the least technological progress sees constant rising emissions to a level as high as 951 Mton in 2060. On the contrary, the scenario with the deepest cost reduction features a distinct pathway in which the emissions drop to 43 Mton in 2060. Interestingly, this low amount of emissions is very close to the carbon-neutral scenario, which has a carbon constraint of 35 Mton in 2060.

In comparison, the constraints put on emissions in the carbon-neutral scenario bend down the curve after 2030. The emissions peak at 428 Mton in 2030 in the deterministic case. Because the emission constraints are effective in the model for many cases, many overlapped pathways are characterized by a very smooth declining trend from 2030 to 2060. In particular, some scenarios have even lower emissions than the constraints after 2040 because high technology progress in these scenarios leads to an optimal strategy putting in place earlier the low-carbon technologies subject to the emissions constraints. For example, the most extreme scenario emits CO2 as low as 87 Mton in 2045, well below the constraint. Earlier in-place of these new technologies would bring about significant reductions in cumulative emissions til the end of the horizon.

5.2. Hydrogen production mix

The distinct emissions pathways result from hydrogen production technology mixes. An instinctive explanation for the scenarios with lower emissions is that renewable-based hydrogen production, or green hydrogen, dominates the mix because of the competitiveness it gained from a further cost reduction of the related technologies. Fig. 5 compares the hydrogen production mix in the two deterministic cases of baseline and carbon-neutral scenarios, including coal-based (H2_coal), natural gas-based (H2_SMR), and water electrolysis with renewable electricity (H2_elec). Note that the coal and SMR routes are divided into two subgroups depending on whether CCS is installed (with the suffixes _CCS and w/o_CCS, respectively). Fig. 6 shows the outputs from these technologies across all the simulated cases covering a wide range of technological progress uncertainty.

The results show that driven by the increases in final product demands, there is a substantial growth in total hydrogen production from 33.4 Mton in 2030 to 72.7 Mton in 2060 across all the scenarios. The share of renewable-based electrolysis (H2_elec) increases in both of the two deterministic cases but at different rates. Under the carbon constraints in the carbon-neutral scenario, the output from this technology rises much faster to 49.9 Mton in 2060, accounting for 69 % of total hydrogen production. This growth rate is roughly half of the baseline. Despite the slower increasing speed, the electrolysis route contributes 34 % to total hydrogen production in the baseline, only second to the coal-based technology. Even though there is no emission constraint in the baseline, the overall cost of this route could gain competitiveness due to technological improvement. In addition, this route has no fuel cost, which also gains some economic advantage over other fossil fuel-based routes.

In the deterministic case of the baseline scenario, the production cost of coal-based, SMR and electrolysis-based hydrogen is 5509, 9145, and 5631 yuan/ton on average over the entire horizon, respectively. The carbon-neutral scenario increases costs to 6006, 9435, and 5861 yuan/ton, respectively, indicating a significant difference in the incremental cost for the three routes. Notably, the most carbon-intensive coal route has the highest incremental cost in the carbon-neutral case, resulting in a declining trend of its share in the production mix.

Note: Each pair of stacked bars represents the deterministic cases of the baseline (left side) and the carbon natural scenario (right side), respectively. The error line on the top of each bar indicates the uncertain range.

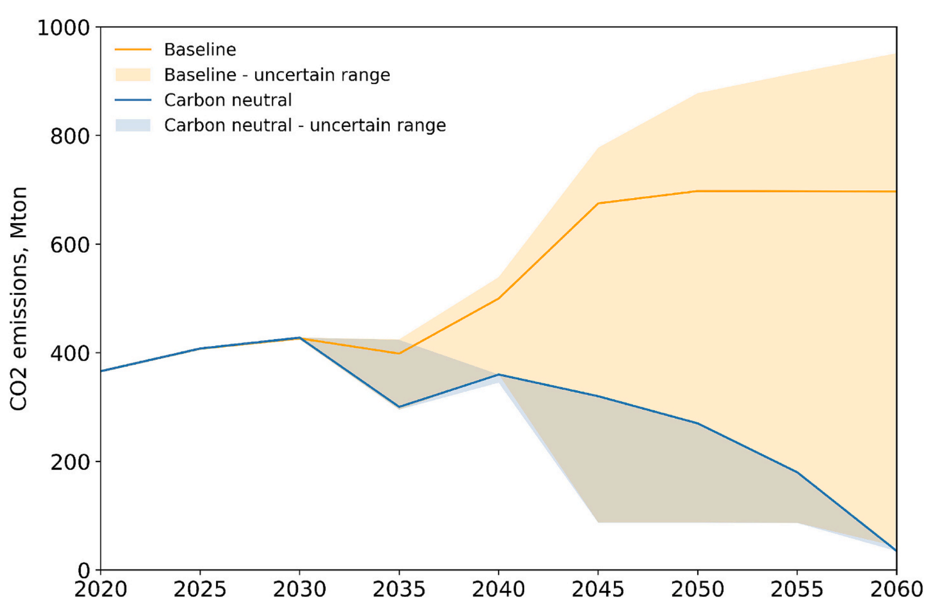

Fig. 4. Projected CO_2 emissions from the hydrogen energy system.

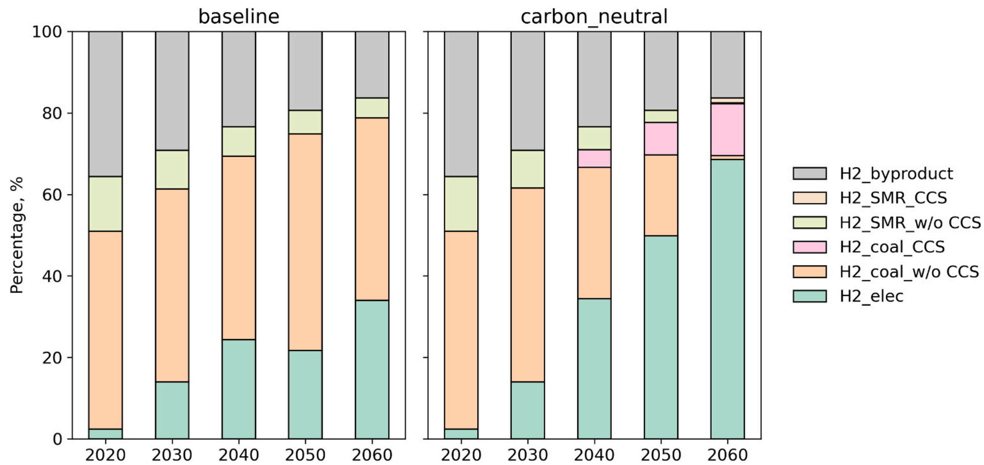

Fig. 5. Hydrogen production mix in the baseline and the carbon neutral deterministic scenarios.

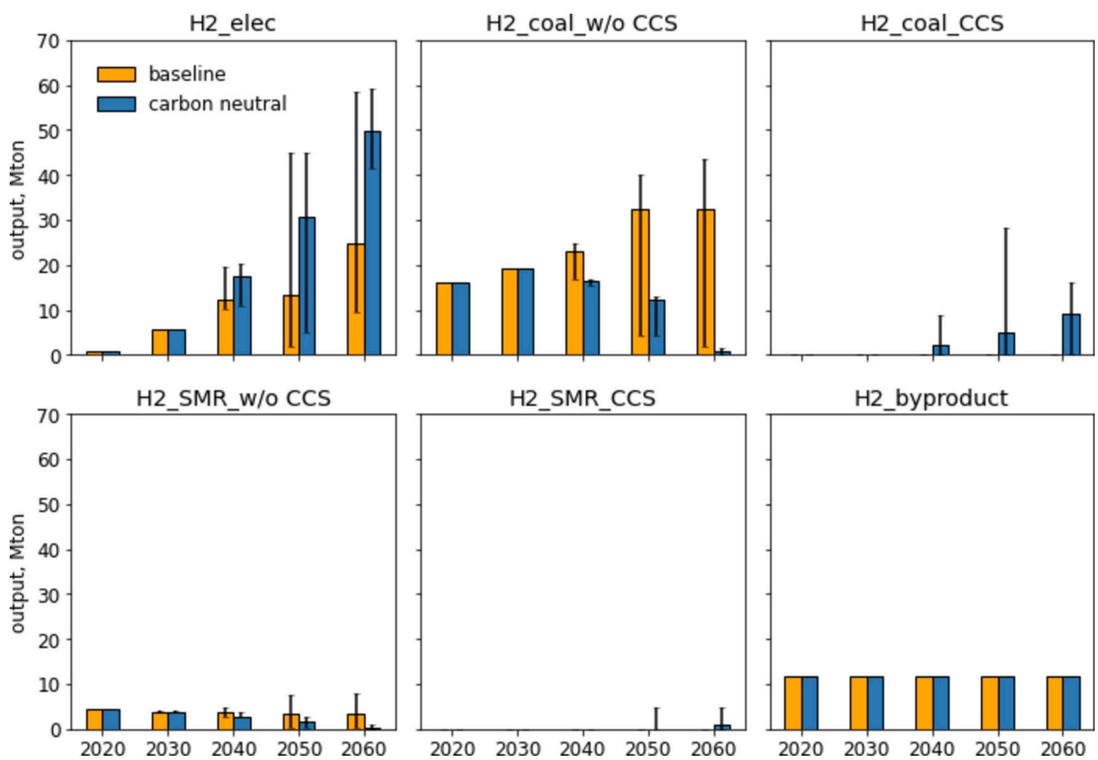

Fig. 6. Projected hydrogen production from different technologies.

Despite the challenge from cost-declining green hydrogen, coal gasification without CCS (H2_coal_w/o CCS) remains the dominating technology in the baseline, where its share remains rather stable at a level of 45–48 % over the whole timespan. It contributes the largest part of total CO2 emissions from the whole energy system. To meet the strict emissions cap constraints in the carbon-neutral case, the coal-based route is gradually phased out, and only a small portion of the coal-based capacities are retained and equipped with CCS installations (H2_coal_ccs). The SMR route output declines in both cases because of the high cost of natural gas as the feedstock. Hydrogen production as a byproduct from other industrial sources is assumed to be constant over time.

Considering all the possible future cost variations, these results show a wide range of uncertainty, particularly for the cases in the baseline. In some cases, with rapid technological advancement, innovative hydrogen production, represented by the electrolysis route, could replace a large amount of the coal-based route and contribute a share as high as 78 % to the total hydrogen supply. This also explains the extremely low emission pathways in some baseline cases even without emission constraints, as shown in Fig. 4. In contrast, the results of the carbon-neutral scenarios show a much smaller uncertain range. The comparison indicates that despite high uncertainty in technology costs, renewable-based hydrogen production should be enhanced and become the dominant technology in the hydrogen supply system. Additionally, CCS is also significant for decarbonizing the remaining coal installations despite the inevitable declining trend of coal-based production.

Fig. 7 presents the results of the final products, represented by ammonia and methanol for simplicity, with different hydrogen feedstocks. As hydrogen production is the main process in producing these downstream products, their energy consumption, carbon emissions, and production mixes are largely affected by the adoption of upstream hydrogen production technologies. Similarly, coal-based production increases its share of both ammonia and methanol in the baseline; green hydrogen-derived products also grow in absolute amounts. However, they only gain the dominant advantage in the carbon-neutral scenarios. The other two, using gas-based and byproduct hydrogen as the feedstock, take a relatively small share in the mixes.

5.3. Capacity expansion and investment

Transitioning the hydrogen energy system requires enormous new capacities and associated investments. Fig. 8 shows the results for cumulative newly installed capacities and the associated investments in different technologies in the system. The dot-connected lines with deep color represent the deterministic cases in both scenario sets, while the light-colored lines show the results for the remaining uncertain scenarios. For renewable electricity generation, it appears that solar PV is favored over wind farms in both scenario groups, as it also enjoys lower capital costs and O&M costs. The solar PV installations reach 134 and 235 GW in the two deterministic cases of the baseline and the carbon neutral scenarios, respectively, corresponding to investments as high as 398 and 671 trillion yuan. This is the single technology with the largest investment in the supply chain. Combined with wind farms and electricity storage, the whole renewable electricity generation system requires a substantial amount of investment that accounts for roughly 78–82 % of the total accumulated investments for the entire hydrogen energy system. The electrolysis capacity in hydrogen production would need 112 (ranging from 63 to 222) and 204 (ranging from 139 to 233) trillion yuan of investment for the baseline and the carbon neutral scenario, respectively. The CCS installations, only appearing in the carbon neutral scenarios, would need 15 trillion yuan of investment (ranging from 0 to 19), taking a relatively small share in the total investment mix.

6. Conclusion and discussions

This study performs a holistic system analysis accounting for uncertain technological advancement through a hybrid modeling approach. The model results reveal some interesting findings concerning the hydrogen energy system transition.

First, the study reveals that without a policy constraint, the CO_2 emissions from China's hydrogen energy system could not peak until 2060, the targeted year for carbon neutrality in the national goal, in many cases with small technology advancement, not to mention reach zero emissions. Nevertheless, speeding up technological progress would bring about significant mission reductions that, even in the baseline, the emissions could drop to a very low level close to the carbon-natural scenarios in 2060. That being said, the carbon neutral goal could be almost achieved automatically without a forced emission cap on the condition of fast technological advancement of crucial technologies.

Second, it is found that green hydrogen capacities would increase in all the scenarios regardless of various cost decline speeds, as it is anticipated that the renewable-based technologies in the hydrogen supply chain will have substantial potential for cost reduction in general. This gives a significant cost advantage for green hydrogen production as this technological route features zero fuel cost besides the low-carbon characteristic. Without an emission reduction requirement in the baseline scenarios, coal gasification without CCS remains the dominant technology, with a rather stable range of 45–48 % over the whole timespan, making it the single largest emission source in the system. To meet the strict emissions cap constraints in the carbon-

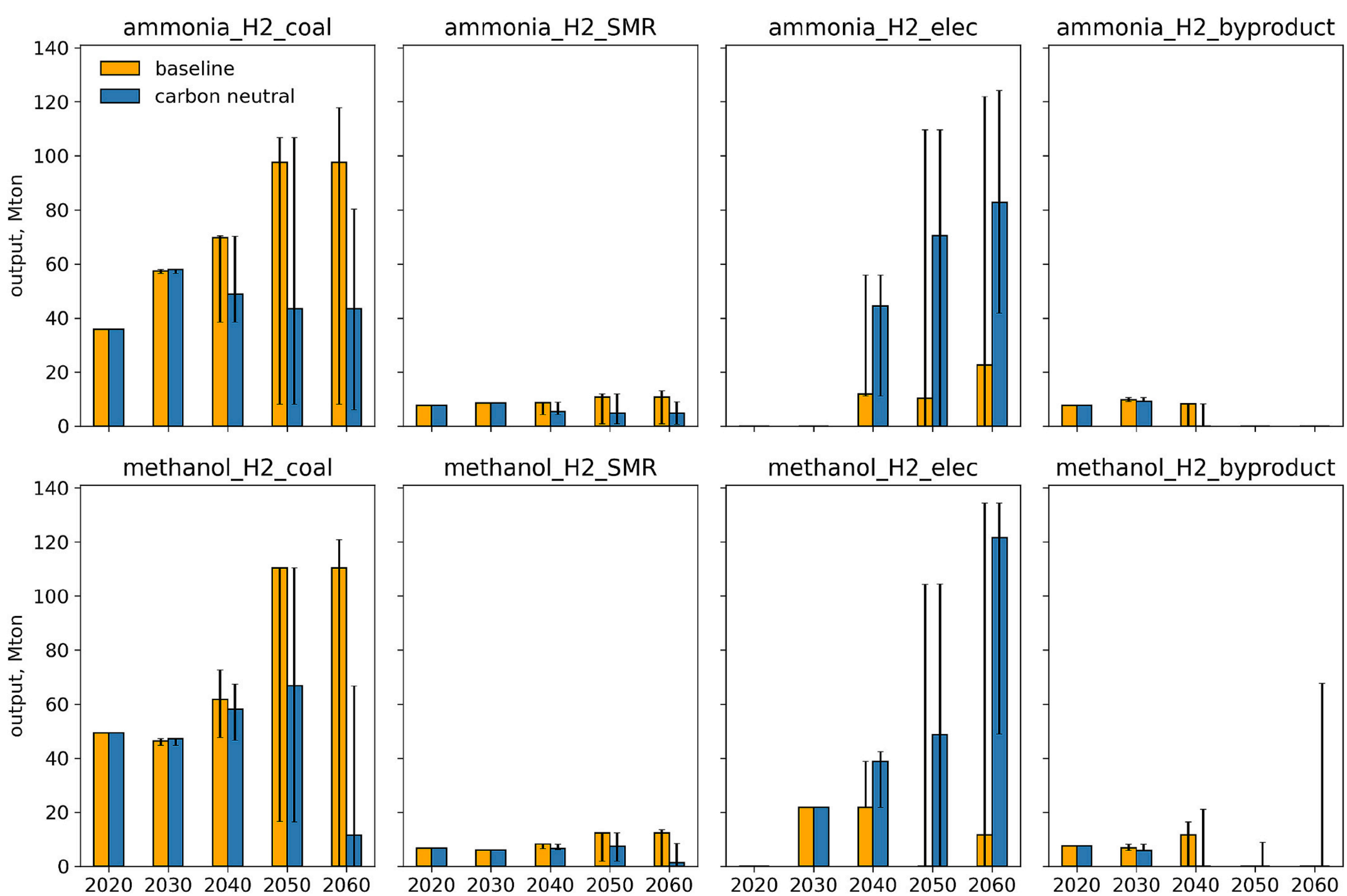

Fig. 7. Projected outputs of ammonia and methanol from different hydrogen sources.
Note: Each pair of stacked bars represents the deterministic cases of baseline (left side) and the carbon natural scenario (right side), respectively. The error line on the top of each bar indicates the uncertain range of the result.

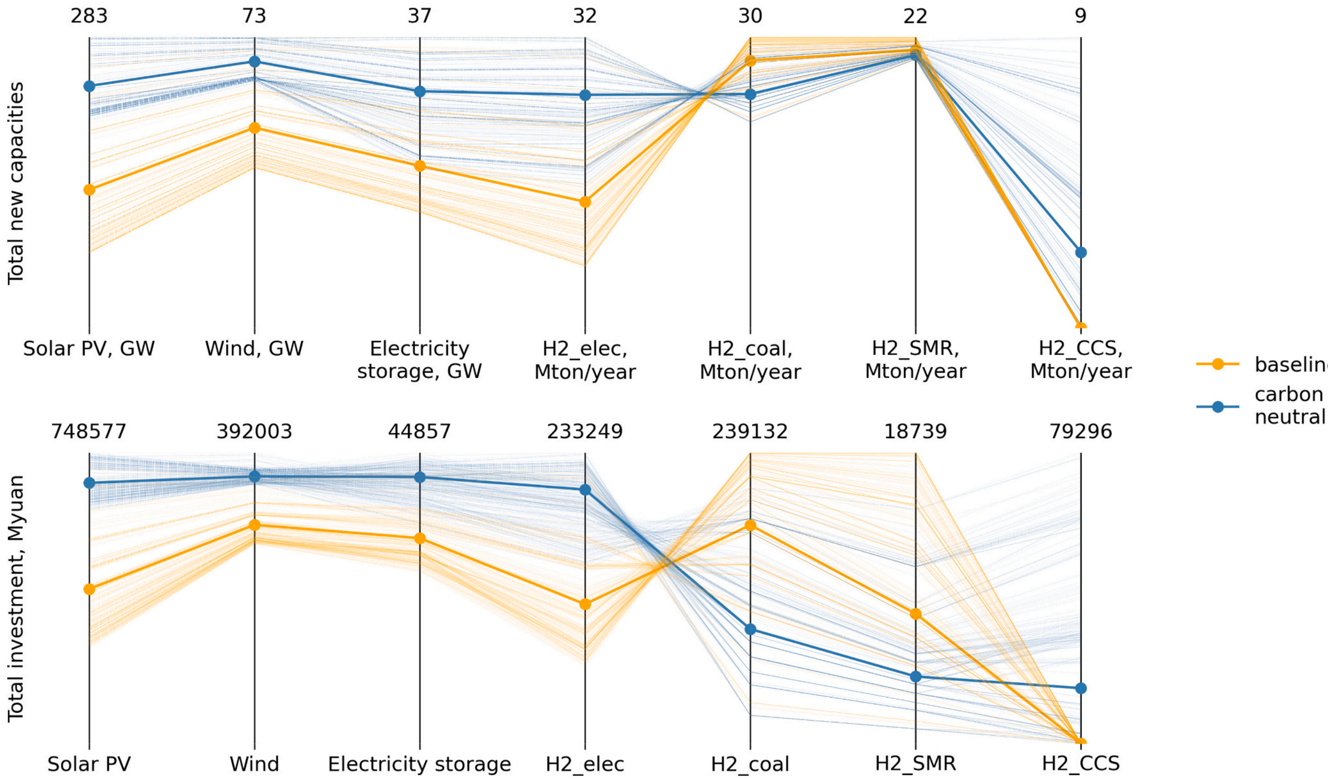

Fig. 8. Accumulated new capacities and investment for different technologies.
Note: H2_coal and H2_SMR refer to the technologies without CCS, and H2_CCS involves all the CCS-related technologies, including both the coal-based and SMR technologies equipped with CCS.

neutral cases, renewable-based green hydrogen dominates the mix. At the same time, the coal-based route is gradually phased out, and only a small portion of these capacities are retained and equipped with CCS installations.

The compositions of the hydrogen production mix largely impact the carbon footprints of some downstream products, such as ammonia and methanol, as hydrogen is the main feedstock for these products. Although not explicitly modeled in this study, other industrial sectors that could use hydrogen as a clean fuel or feedstock would have similar impacts. For instance, using hydrogen to replace coke or natural gas is one of the most important solutions in decarbonizing the iron and steel industry. However, this study suggests that unless hydrogen is produced from renewable electricity, the downstream use of hydrogen could also cause fast increases CO2 emissions upstream, as shown by the baseline results in the model calculations.

Another important finding is that technological progress in renewable electricity supply is the key to accelerating the transition to a green hydrogen energy system. Renewable energy, such as solar PV and wind farms, and electricity storage, account for a substantial amount of investment needed by installing the green hydrogen supply chain. Enabling a deep transformation of the hydrogen system implies enormous capital investment into innovative technologies. The fast development of renewable energy has led to a significant reduction in renewable electricity costs. Many countries have also set ambitious goals for renewable energy development, most of which are limited to the electricity sector.

Key policy implications could be drawn from the results regarding subsidies, carbon pricing, and infrastructure development to foster the development of hydrogen technologies. Governments can provide subsidies to incentivize the adoption of hydrogen technologies, particularly in the early stages of market development. However, subsidies should be designed to phase out as the market matures and complement other policy measures to ensure long-term sustainability. Moreover, implementing a carbon pricing mechanism, such as the ongoing national emissions trading scheme (ETS), can create a financial incentive for industries to adopt cleaner technologies; it is suggested that hydrogen-related industries should be included in the national ETS as soon. In addition, there is a need for substantial investment in infrastructure, including production facilities, storage, and distribution networks. Such an infrastructure should be compatible with existing energy systems and can support the large-scale deployment of hydrogen technologies. It, therefore, requires an elaborate and systematic policy design to integrate hydrogen into the broader energy policy landscape.

CRediT authorship contribution statement

Wenji Zhou: Writing – review & editing, Writing – original draft, Methodology, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Hongtao Ren:** Writing – review & editing, Writing – original draft, Supervision, Software, Methodology, Investigation, Funding acquisition, Conceptualization. **Xiao-Bing Zhang:** Writing – review & editing, Writing – original draft, Resources. **Shuai Shao:** Writing – review & editing, Writing – original draft, Validation, Funding acquisition.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.eneco.2024.108135.

Data availability

The key data regarding technological costs and other parameters in the mode are provided in its supplementary materials; other data supporting this study's findings are available upon reasonable request.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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