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A Multi-Level Uncertainty Conduction Model for Synergistic Pollution and Carbon Mitigation in the Yellow River Basin Coal Chemical Industry

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Abstract

This study focuses on the multi-dimensional uncertainties in synergistic pollution reduction and carbon mitigation pathways for the coal chemical industry in the Yellow River Basin, a region facing extreme water scarcity (only 2% of national water) and fragile ecology, and constructs a Multi-Level Uncertainty Conduction (MLUC) Model integrating data, modeling, and validation. Using 2011–2025 data, Monte Carlo (10,000) simulations quantify the impacts of policy, technology, market, and ecological uncertainties on synergistic benefits. Sobol' global sensitivity (Saltelli) and Shapley decomposition (14 technologies) identify key drivers and technology contributions. A system dynamics model simulates 2023–2050 pathways under baseline, policy-enhanced, technology breakthrough, and composite uncertainty scenarios. Logarithmic Mean Divisia Index (LMDI-I) decomposition reveals a six-factor driving mechanism for carbon emission changes. Results show that policy uncertainty exerts the largest influence, with a variance contribution of approximately 35%, followed by technology (28%), market (22%), and ecological factors (15%)—the latter primarily reflecting water availability and regional ecological carrying capacity. Critical thresholds are 80 CNY/t CO₂ for carbon capture, utilization and storage (CCUS) viability, and 6.8 CNY/t for green hydrogen substitution. Comprehensive resource utilization is optimal near term, while green hydrogen substitution and CCUS–green hydrogen coupling dominate medium- to long term. The proposed dynamic threshold response mechanism and technology portfolio strategy could boost synergistic benefits by 22% to 35%. These findings underscore the need for watershed-scale collaborative governance and integrated water–carbon–energy management to ensure robust mitigation under the basin's constraints.



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Keywords: Yellow River Basin; coal chemical industry; pollution reduction and carbon mitigation; uncertainty analysis; MLUC Model

1. Introduction

The Yellow River Basin is a critical energy production and processing hub in China, holding 472 billion tonnes of coal reserves, which account for 47% of the national total [1]. Major coal chemical bases such as Ningdong, Ordos, and Yulin have been established within the basin, and in 2023, its coal chemical output constituted roughly 60% of China's

production [2], with carbon emissions reaching 1.26 billion tonnes, representing 22% of national industrial emissions [3]. However, the basin possesses only 2% of the country's total water resources [4], yet it hosts approximately 60% of the national capacity in the highly water-intensive coal chemical industry, intensifying the conflict between industrial development and ecological constraints. Against the backdrop of ecological protection and high-quality development of the Yellow River Basin being elevated to a national strategy, achieving synergistic governance of pollution reduction and carbon mitigation in the coal chemical industry within a basin characterized by extreme water scarcity and a fragile ecological foundation has become an urgent scientific and policy challenge.

Research on industry-specific pathways for pollution and carbon reduction has advanced the assessment of synergistic effects [5–7]. Many studies quantify these effects using coupling coordination models, cross elasticity methods, and data envelopment analysis (DEA) frameworks [7–10]. Others evaluate the economic viability of technological pathways based on marginal abatement cost and cost benefit frameworks [11–13], while additional research employs numerical simulation and econometric models to analyze policy and regional differences [8,14]. However, current methods largely rely on deterministic assumptions and thus fail to capture how dynamic uncertainties such as policy shifts, technological change, and market fluctuations affect synergistic benefits.

On the other hand, current research lacks a unified conceptual definition or measurement framework for uncertainty, and most studies are confined to a single industry or a single dimension [15–17]. Lo Piano and Benini (2022) systematically reviewed the shortcomings of uncertainty and sensitivity analysis methods in life cycle assessment [15]. Habibi et al. (2023) summarized uncertainty modeling approaches for biofuel supply chains [16]. Chen et al. (2024) found that supply chain research is shifting from single uncertainty to multi-dimensional and multi-objective decision making, yet the field remains underdeveloped overall [17]. At the watershed scale, quantitative coupling of the four dimensions of policy, technology, market, and ecology is still missing. The transmission mechanisms between systems and the coupling effects of multi-dimensional uncertainty urgently need further exploration.

To address the above research gap, this study proposes a multi-level uncertainty propagation model that integrates three analytical frameworks: the Driving Force–Pressure–State–Impact–Response (DPSIR) driver mechanism [18,19], complex system feedback loops, and the policy technology market triple helix [20,21]. The model systematically characterizes how uncertainty propagates through the driver, pressure, state, impact, and response stages, along with their superimposed effects. Methodologically, we introduce an interdisciplinary combination of Monte Carlo simulation, Sobol global sensitivity analysis, Shapley value cooperative game decomposition, system dynamics simulation, and Logarithmic Mean Divisia Index (LMDI) decomposition. This forms a closed loop research pathway from data collection and status diagnosis to uncertainty modeling, scenario simulation, and strategy optimization. This paper aims to answer two core questions. Under the stringent water resource and ecological constraints of the Yellow River Basin, how do multi-dimensional uncertainties affect the effectiveness and robustness of synergistic pollution and carbon reduction pathways in the coal chemical industry? And how can dynamic strategy design maximize synergistic benefits under uncertain conditions?

2. Materials and Methods

2.1. Research Framework and the MLUC Model

We constructed a closed loop research pathway from data collection and status diagnosis to uncertainty modeling, scenario simulation, and strategy optimization, as shown in Figure 1. To systematically characterize multi-dimensional uncertainty in the synergistic

pollution and carbon reduction pathway, we propose the multi-level uncertainty propagation model, or MLUC. The model relies on three core mechanisms. First, the DPSIR driver mechanism embeds carbon and pollutant emissions from the coal chemical industry into the watershed ecology, economy, and social system. It traces how uncertainty propagates from driver, pressure, state, impact to response. Driver represents economic development and energy demand. Pressure represents carbon and pollutant emissions. State represents environmental quality and ecological carrying capacity. Impact represents climate change and public health. Response represents policy intervention and technology deployment. Second, the complex system feedback loop captures positive and negative feedbacks among four subsystems: industrial development, pollution emissions, carbon cycle, and policy regulation. For instance, a carbon price increase raises production costs, suppresses output, and reduces carbon emissions, forming a negative feedback loop. Conversely, technological progress lowers costs, stimulates output expansion, and increases carbon emissions, forming a positive feedback loop. These two loops alternate dominance across different time scales. Third, the triple helix of policy, technology, and market denotes that policy drives technology deployment, technology reshapes market structure, and market feedback in turn influences policy adjustment. Together, they form a spiraling co-evolutionary relationship. The MLUC model uses Monte Carlo simulation to quantify the superimposed effects of these mechanisms on synergistic benefits.

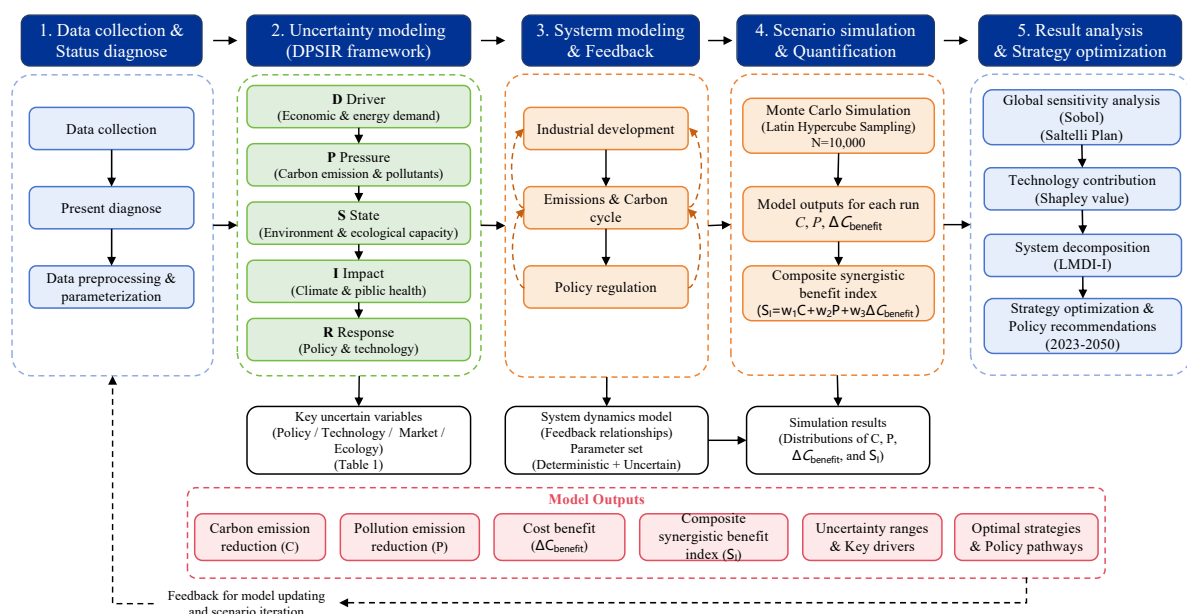


Figure 1. Research technical framework.

2.2. Data Sources

The research data cover the coal chemical industry across nine provinces and regions in the Yellow River Basin, specifically Shanxi, Inner Mongolia, Shandong, Henan, Sichuan, Shaanxi, Gansu, Qinghai, and Ningxia. Eight subsectors are included as follows: coal-to-coke, synthetic ammonia, methanol, ethylene glycol, natural gas, direct coal to oil, indirect coal to oil, and olefins. The time span extends from 2011 to 2050. Data sources include the *China Statistical Yearbook*, ecological and environmental statistics, statistical records of coal chemical bases within the basin, the industry catalog of recommended energy-saving technologies, the catalog of industrial water saving technologies and equipment, and research papers [3,22–34]. A detailed data inventory is provided in the Supplementary Materials, Tables S1–S6.

2.3. Synergy Evaluation System

The synergistic benefit is evaluated using a three dimensional weighted composite index:

$$S_I = 0.4 \times C + 0.3 \times P + 0.3 \times \Delta C_{\text{benefit}} \quad (1)$$

where C represents the carbon emission reduction potential (10^4 t CO_2), P represents the pollutant emission reduction potential (10^4 t pollutant equivalent), and $\Delta C_{\text{benefit}}$ denotes the net cost benefit (10^4 CNY), with the pollutant equivalent conversion performed in accordance with the Environmental Protection Tax Law of the People's Republic of China [22]. The pollutant equivalent aggregates twelve pollutants: ammonia (NH_3), ammonia nitrogen ($\text{NH}_3\text{-N}$), nitrogen oxides (NO_x), sulfur dioxide (SO_2), chemical oxygen demand (COD), volatile phenol (VP), volatile organic compounds (VOCs), particulate matter (PM), cyanide (CN), petroleum pollutants (PPs), total nitrogen (T-N), and total phosphorus (T-P). Carbon emission accounting covers direct and indirect emissions from three sources: raw material consumption, fuel combustion, and electricity and heat. Conversion factors and the detailed assessment system are provided in Table S5.

2.4. Uncertainty Analytical Framework

Based on the DPSIR model [35,36], the uncertainty system is divided into four dimensions: policy, technology, market, and ecology. Key variables and their probability distribution types are summarized in Table 1. The complete distribution characteristics of each parameter, such as the minimum, mode, and maximum of the triangular distribution for carbon price and the location parameter μ and the scale parameter σ of the lognormal distribution for green hydrogen cost, are detailed in Table S7 in the Section S2.2 of the Supporting Materials.

Table 1. Key variables of four dimensional uncertainties based on DPSIR.

DPSIR Component	Uncertainty Dimension	Key Variable	Distribution Type
Driver (D)	Policy	Carbon price	Triangular distribution
		Policy Stringency increase frequency of emission standards	Poisson distribution
		Policy intensity coefficient for technology promotion	Uniform distribution
Pressure (P)	Technology	Carbon capture, utilization and storage (CCUS) cost	Normal distribution
		Technology Green hydrogen cost	Lognormal distribution
		Technology Fluctuation in technology penetration rate	Uniform distribution
State (S)	Market	Coal price volatility	Normal distribution
		Market Product demand elasticity	Uniform distribution
		Market Electricity carbon emission factor	Normal distribution
Impact (I)	Ecology	Water availability coefficient	Gamma distribution
		Ecology Frequency of extreme climate events	Poisson distribution
Response (R)	Technology–policy coupling	Energy efficiency decay rate	Beta distribution

2.5. Model Construction

2.5.1. Monte Carlo Uncertainty Quantification

Latin Hypercube Sampling (LHS) [37] was employed to perform 10,000 simulations, thereby propagating parameter uncertainty. For each sample, carbon emission reduction (C), pollutant emission reduction (P), and net cost benefit ($\Delta C_{\text{benefit}}$) were calculated sequentially, and a composite synergistic benefit index was synthesized from these three objective functions. The net cost benefit integrates the monetized values of carbon reduction gains, quantified as the carbon price multiplied by carbon emission reductions, and pollutant reduction gains, derived from pollution charge savings or avoided environmental damage costs. Statistical analysis of the 10,000 simulation outcomes yielded the probability distribution, selected quantiles, and variance contribution rate of the index.

$$C = \sum_{ij} (E_{ij} \times \Delta P_{ij} \times \theta_{ij}) \quad (2)$$

$$P = \sum_{ij} (F_{ij} \times \Delta P_{ij} \times \varphi_{ij}) \quad (3)$$

$$\Delta C_{\text{benefit}} = \sum_{ij} (B_{ij} - C_{\text{fixed},ij} - C_{\text{operating},ij}) \quad (4)$$

where i denotes the subsector index ($i = 1, 2, \dots, 8$), corresponding to coal-to-coke, synthetic ammonia, methanol, ethylene glycol, natural gas, direct coal liquefaction, indirect coal liquefaction, and olefins, respectively. j is the reduction technology index ($j = 1, 2, \dots, 14$), with technology names and codes detailed in Section S2.4 of the Supporting Materials. E_{ij} , F_{ij} , and B_{ij} represent the carbon emission reduction potential (10^4 t CO₂), pollutant emission reduction potential (10^4 t pollutant equivalent), and reduction benefit (10^4 CNY) for subsector i when technology j achieves its maximum penetration rate. ΔP_{ij} denotes the change in the penetration rate of technology j in subsector i (%). θ_j and φ_j are dimensionless correction factors for the carbon reduction effectiveness and pollutant reduction effectiveness of technology j , respectively. $C_{\text{fixed},ij}$ and $C_{\text{operating},ij}$ are the fixed cost and annual operating cost (10^4 CNY) for deploying technology j in subsector i .

2.5.2. Sobol Global Sensitivity Analysis

A global sensitivity analysis was performed on 15 key parameters, including carbon price, CCUS penetration rate, green hydrogen cost, and comprehensive resource utilization penetration rate; it was conducted using the Sobol' method with the Saltelli sampling scheme [38–40]. Detailed parameter ranges are given in Table S8 in the Section S2.3 of the Supporting Materials. The base sample size N was set to 1024, yielding a total of 32,768 model evaluations. The first-order index (S_{1i}) and total-effect index (S_{Ti}) were computed to quantify the main effect and interaction effect of each parameter, respectively. A parameter was deemed to exert a significant influence if $S_{Ti} > 0.1$, and a difference $S_{Ti} - S_{1i} > 0.1$ indicated the presence of significant interactions. Comparison of multi-level sensitivity analysis methods are shown in Table S9.

$$S_{1i} = V[E(Y|X_i)]/V(Y) \quad (5)$$

$$S_{Ti} = 1 - V[E(Y|X_{-i})]/V(Y) \quad (6)$$

where $V(Y)$ represents the total variance of the model output Y , $V[E(Y|X_i)]$ is the variance of the conditional expectation of Y given parameter X_i , X_{-i} denotes the set of all parameters other than X_i , and $V[E(Y|X_{-i})]$ is the variance of the conditional expectation of Y given all parameters except X_i .

2.5.3. Shapley Value-Based Technology Contribution Analysis

We treated the 14 mitigation technologies as players in a cooperative game, with the total synergistic benefit serving as the coalition payoff. By exhaustively enumerating all 2^{14} (16,384) technology combinations, we computed the Shapley value φ_i for each technology [41]. A synergy factor δ was introduced to quantify the coupling gains among technologies. To reveal the dynamic evolution of technology contributions, we calculated the Shapley values for the years 2025, 2030, and 2050. The complete technology list and groupings are provided in Tables S10–S12 in the Section S2.4 of the Supporting Materials.

$$\varphi(i) = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|!(14 - |S| - 1)!}{14!} [v(S \cup \{i\}) - v(S)] \quad (7)$$

$$v(S) = \omega_c C_S + \omega_p P_S + \omega_{\text{cost}} \Delta C_S \quad (8)$$

$$\delta = 1 + 0.05(|S| - 1) \quad (9)$$

where S denotes any subset of technologies that excludes technology i , referred to as a coalition. $|S|$ is the number of technologies in the coalition, ranging from 0 to 13. $v(S)$ is the characteristic function value of coalition S , representing the total synergistic benefit generated by that technology combination. The term $v(S \cup \{i\}) - v(S)$ quantifies the marginal benefit increment when technology i joins coalition S . In the calculation, C_S and P_S are the total carbon emission reductions (10^4 t CO₂) and total pollutant reductions (10^4 t equivalent) when all technologies in combination S are deployed synergistically, and ΔC_S is the net cost benefit of combination S (10^4 CNY). The weighting coefficients w_c , w_p , and w_{cost} are set at 0.4, 0.3, and 0.3, respectively, consistent with the composite synergistic benefit index.

2.5.4. System Dynamics Simulation

A system dynamics model [42] was built to simulate the dynamic trajectories of carbon and pollutant emissions from 2023 to 2050. The model integrates four subsystems: industrial development, pollution emission, carbon cycling, and policy regulation. It incorporates two key feedback mechanisms. The first triggers a rapid scale-up of CCUS carbon capture once the carbon price surpasses the threshold of 80 CNY per tonne of CO₂ [43–45]. The second assumes that the penetration rate of each technology follows a logistic S-curve diffusion process [46,47], with the inflection year set according to the technology's maturity level. The model runs on an annual time step, tracking state variables such as carbon emissions, pollution equivalents, production capacity structure, and carbon price. Further details on the numerical integration can be found in Table S13 in the Section S2.5 of the Supporting Materials.

2.5.5. Scenario Design

We developed four contrasting scenarios. The Business-as-Usual (BAU) scenario maintains current policy trends, with the carbon price rising slowly to approximately 111 CNY per tonne by 2050 and technologies diffusing at their natural pace. The Enhanced Policy Scenario (ESP) is predicated on resolute progress toward the dual-carbon goals, featuring a carbon price that reaches around 299 CNY per tonne and technology deployment accelerated by 5 to 10 years relative to the BAU. The Technology Breakthrough Scenario (TBS) assumes that green hydrogen cost falls below the critical threshold of 6.8 CNY per kg, CCUS costs drop by 50% from current levels, and the penetration rate of green electricity increases substantially. The composite uncertainty scenario (CUS) pushes multi-dimensional uncertainties to extremes, with carbon prices surging rapidly to about 386 CNY per tonne while the progress of certain technological breakthroughs remains highly uncertain. Key parameter comparisons across scenarios are presented in Table 2, and

detailed technology penetration rate settings are provided in Table S14 in the Section S2.5 of the Supporting Materials.

Table 2. Comparison of key parameters across the four scenarios.

Parameter	BAU	ESP	TBS	CUS
Carbon price in 2023 (CNY/t)	50	80	60	80
Carbon price in 2050 (CNY/t)	~111	~299	~173	~386
Carbon price annual growth rate	3%	5%	4%	6%
Annual decline rate of traditional capacity	2%	3%	2.50%	3.50%
Annual growth rate of modern capacity	3%	4%	5%	2%
Green hydrogen, CCUS, and green electricity penetration rate (2050)	25%	50%	75%	50–75%
Inflection year of technology diffusion	2035	2030	2028	2030–2040

2.5.6. Multi-Objective Optimization

We developed an NSGA-II multi-objective optimization model [48] to identify the Pareto optimal frontier among carbon emission reduction, pollutant reduction, and cost effectiveness, subject to fifteen constraints including capacity limits and technology mutual exclusivity. Details of the model are provided in Section S2.5 of the Supporting Materials. Current carbon and pollutant emission levels and the synergistic benefit weights are presented in Section S2.1 of the Supporting Materials. A multi-level methodological framework was adopted, comprising local sensitivity analysis, Sobol' global sensitivity analysis, Shapley value decomposition, and Monte Carlo variance decomposition. A comparison and description of these methods can be found in Section S2.5 of the Supporting Materials.

3. Results

3.1. Current Status of Pollution and Carbon Emission

In 2023, carbon emissions from the coal chemical industry in the Yellow River Basin accounted for 60% of the sector's national total, with traditional coal chemical processes contributing 62% and 69% of the basin's total carbon and pollutant emissions, respectively [49]. Using the Logarithmic Mean Divisia Index (LMDI-I) method [50], carbon emission changes can be decomposed into six driving factors. Results for the historical period (2011–2023) (Figure 2a) show that the scale effect, i.e., output growth, was the dominant force increasing emissions, cumulatively adding approximately 580 Mt CO₂, while declining energy intensity was the primary mitigating factor, reducing emissions by about 180 Mt CO₂. From 2023 to 2030, the contribution of the technology reduction effect surpassed that of the scale effect for the first time, marking the industry's entry into a decisive phase for carbon peaking. During 2030–2050, the structural effect of shifting from traditional to modern coal chemical processes and the technology reduction effect jointly propelled deep decarbonization (Figure 2b). Meanwhile, the emission reduction contribution from energy structure optimization, particularly green electricity substitution, intensified significantly during the 2040–2050 period.

3.2. Uncertainty Quantification

3.2.1. Monte Carlo Simulation Results

Monte Carlo simulation using Latin Hypercube Sampling (N = 10,000) reveals substantial uncertainty in the synergistic benefits among carbon emission reduction, pollutant reduction, and cost effectiveness for the coal chemical industry in the Yellow River Basin (Figure 3a). Policy-related parameters, such as carbon price and emission standards, account for approximately 35% of the variance contribution, technology-related parameters such as CCUS cost and green hydrogen cost contribute around 28%, while market and

ecological dimensions contribute roughly 22% and 15%, respectively (Figure 3b). Figure 3 also illustrates that when the carbon price surpasses 80 CNY per tonne, the economic performance of CCUS technology improves significantly, with carbon capture volume exhibiting a nonlinear surge. When the green hydrogen cost drops below 6.8 CNY per kilogram, the contribution of the green hydrogen substitution pathway S1 to synergistic emission reduction benefits can reach 51%.

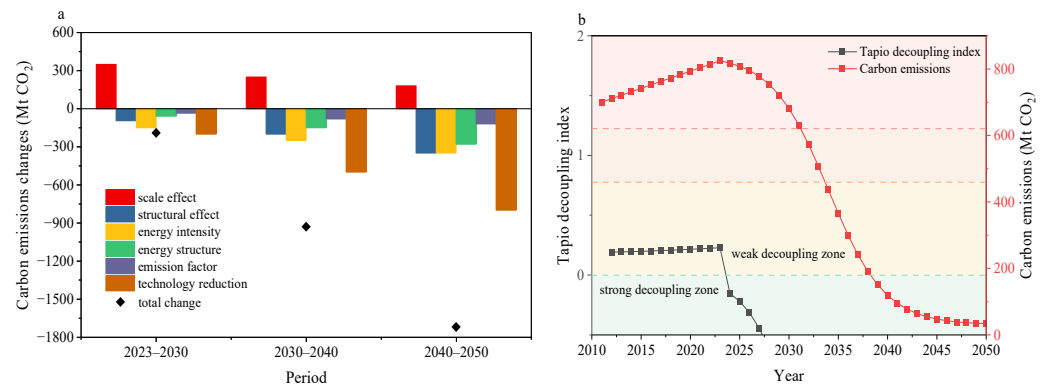


Figure 2. Current status and projections of carbon and pollutant emissions from the coal chemical industry in the Yellow River Basin. (a) Driving factors for changes in carbon emissions in the coal chemical industry; (b) decoupling index of carbon emissions and economic growth in the coal chemical industry (2011–2050).

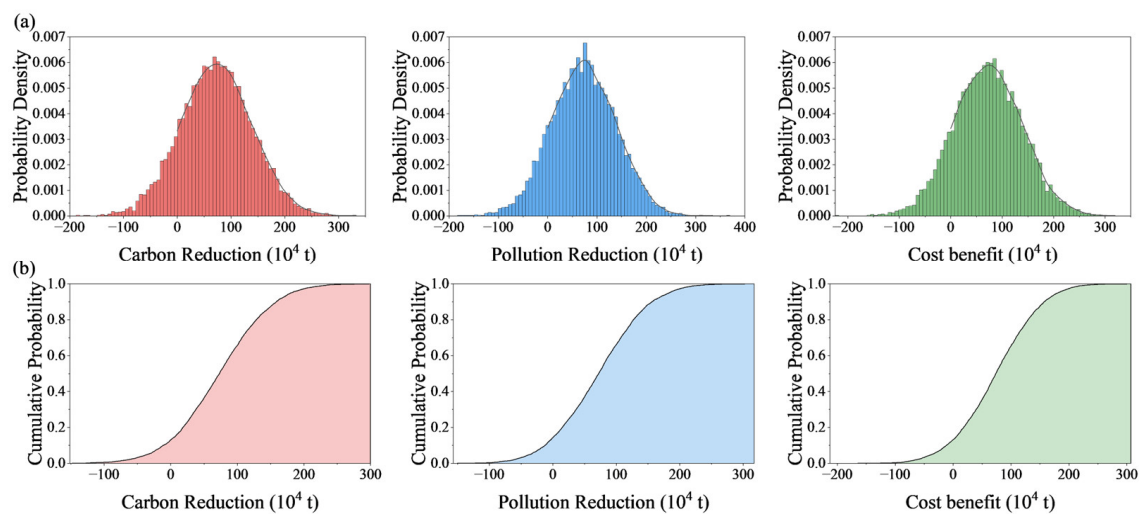


Figure 3. Probability density distribution and cumulative distribution function of synergistic benefits from Monte Carlo simulation. (a) Monte Carlo probability density distribution; (b) Monte Carlo cumulative distribution function curve.

3.2.2. Sobol' Global Sensitivity Analysis

In the Sobol' analysis employing the Saltelli sampling scheme, the base sample size was set to 1024, the number of parameters was 15, and the total sample size was approximately 17,408. The results indicate that the carbon price parameter P1 has the highest total-effect index S_T , making it the primary driver of carbon emission reduction (Figure 4a). The CCUS technology penetration rate parameter P2 and the green hydrogen cost parameter P3 follow closely. For both P2 and P3, the difference between the total-effect index and the first-order index exceeds 0.1, revealing significant interaction effects and suggesting that the coupled deployment of green hydrogen and CCUS yields greater synergistic benefits than promoting either technology in isolation. For the pollutant reduction objective, the comprehensive resource utilization penetration rate parameter P5 and the VOC control policy

intensity parameter P10 exhibit relatively high total-effect indices (Figure 4b). Regarding the cost-effectiveness objective, the carbon price parameter P1 and the coal price fluctuation parameter P7 are the dominant driving factors. Under the long-term 2050 framework, the influence of parameter P13 (the output growth rate of coal-to-olefins) and parameter P14 (the output growth rate of coal-to-synthetic natural gas) intensifies significantly, reflecting the profound impact of modern coal chemical industry expansion on long-term emission reduction pathways.

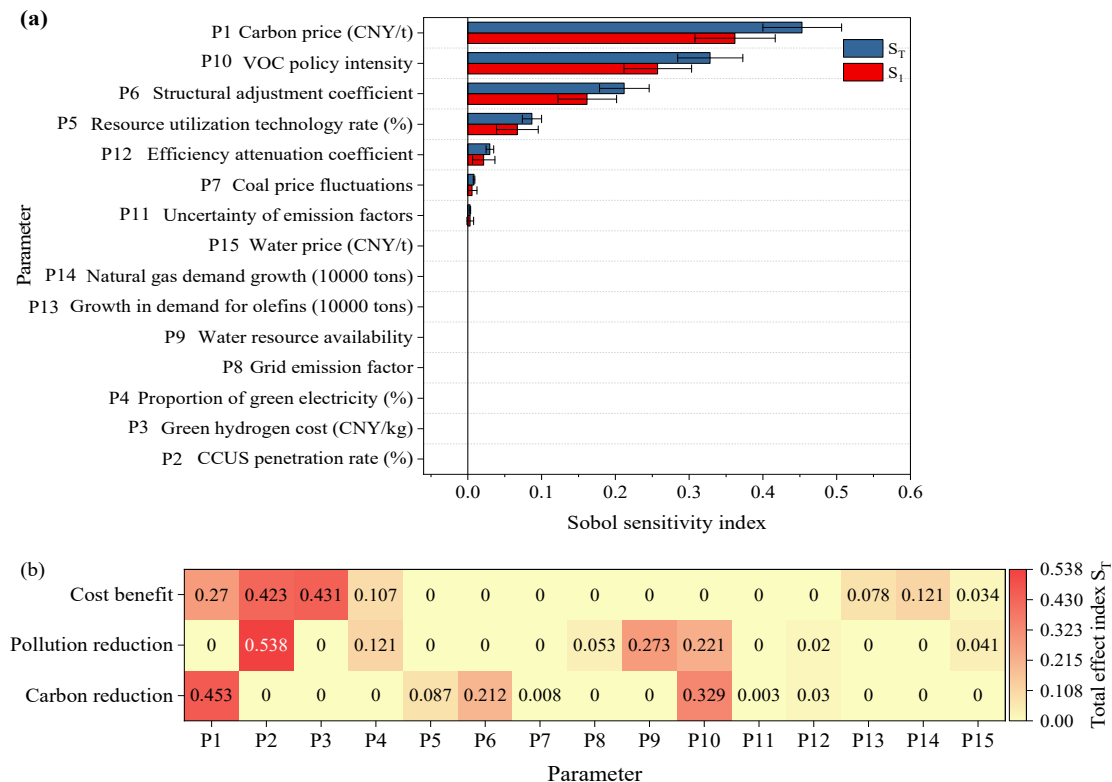


Figure 4. Sobol global sensitivity analysis for carbon emission reduction and comparison of total-effect indices. (a) Global sensitivity analysis of carbon emission reduction; (b) comparison of total-effect index for carbon reduction, pollutant reduction, and cost benefit.

3.2.3. Shapley Value Analysis of Technology Contributions

Applying cooperative game theory, we performed a Shapley value analysis through the exact enumeration of all 16,384 technology combinations to identify the fair marginal contribution of each mitigation technology across different time phases. As shown in Figure 5, comprehensive resource utilization technology (technology R, see Table S5 for its full description) emerges as the largest contributor to synergistic emission reduction in 2025, reflecting the outstanding near-term cost-effectiveness advantage of gasification slag and fly ash utilization. From 2030 onward, the marginal contributions of the CCUS–green hydrogen coupling technology S2 and the green electricity direct supply technology E2 rise progressively. By 2050, the combined contribution of green hydrogen substitution S1, CCUS–green hydrogen coupling S2, and green electricity E2 reaches 72% to 98%, establishing them as the dominant mitigation pathway. This finding corroborates the high total-effect indices of parameters P2, P3, and P4 in the Sobol analysis, lending support to the strategy of progressively scaling up novel low-carbon technology deployment around 2030 and achieving deep application by 2050.

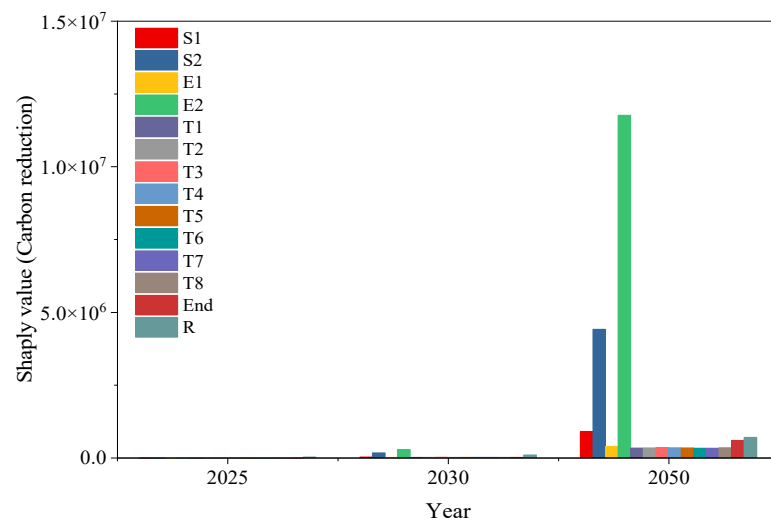


Figure 5. Temporal evolution of Shapley values for individual technologies.

3.3. Scenario Simulation Results

A system dynamics model with an annual time step simulated the dynamic evolution pathways of synergistic carbon and pollutant emission reduction under four scenarios from 2023 to 2050 (Figure 6). Under the BAU scenario, carbon emission reduction grew steadily yet remained insufficient to underpin deep decarbonization, reaching a cumulative total of approximately 577.72 Mt CO₂ by 2050, a result consistent with the baseline scenario reported by Sun et al. (2025) [49]. The ESP scenario demonstrated substantial synergistic mitigation potential between 2025 and 2030; however, the marginal cost effectiveness declined by roughly 12% to 18% relative to the BAU scenario because high-cost technologies such as green hydrogen substitution, CCUS coupling, and end-of-pipe treatment had to be deployed ahead of schedule. In the TBS scenario, once the green hydrogen cost broke below the 6.8 CNY/kg threshold, synergistic benefits climbed rapidly, and the carbon emission reduction in 2050 was approximately 2.9 times that of the BAU scenario. Under the CUS scenario, the distribution interval of synergistic benefits in 2050 was the widest, with the span of carbon emission reduction between the fifth and 95th percentiles reaching $\pm 35\%$, underscoring the compounding effect of multi-dimensional uncertainties.

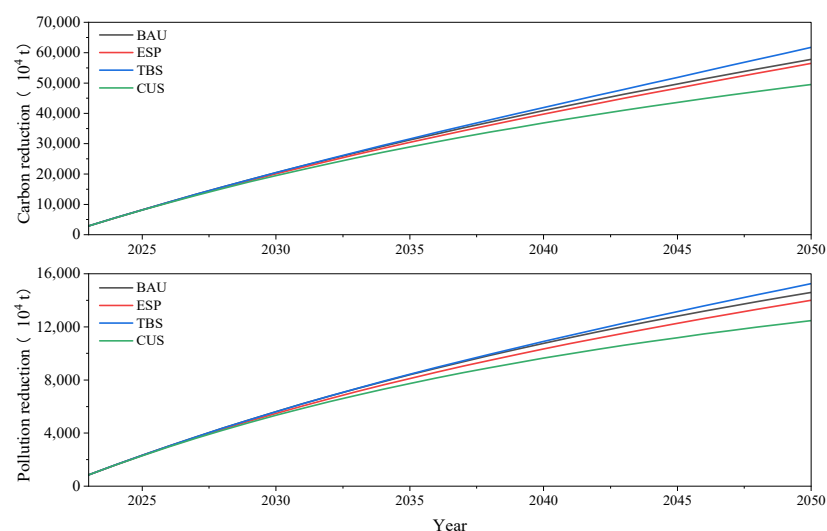


Figure 6. Dynamic evolution of synergistic benefits under the four scenarios.

Regarding the temporal deployment strategy, it is advisable around 2025 to follow the ESP pathway by strengthening the application of comprehensive resource utilization

technologies while simultaneously launching demonstration deployments of green hydrogen substitution, CCUS coupling, and direct green electricity supply. Around 2030, the industry can return to a baseline development rhythm, continuing the large-scale rollout of resource utilization technologies and gradually expanding the engineering application of these novel low-carbon technologies. By 2050, an intensified development strategy should be adopted again to drive innovative breakthroughs and the deep deployment of green hydrogen substitution, CCUS coupling, and direct green electricity supply.

4. Discussion

4.1. Mechanisms of Uncertainty Impact

Both the Monte Carlo simulations and the Sobol analysis consistently indicate that policy uncertainty is the most influential dimension for synergistic benefits, accounting for approximately 35% of the variance, with technological uncertainty following closely at around 28%. The threshold effect of the carbon price is particularly noteworthy: once the carbon price exceeds 80 CNY per tonne, the economic viability of CCUS technology undergoes a structural transformation. This 80 CNY/t critical point is significantly lower than the assessed capture costs for CCUS in China's coal chemical industry [51–53]. The discrepancy primarily arises because our model focuses on high-concentration emission sources, considers only the capture stage cost, and incorporates dedicated subsidies. It should be noted, however, that our estimated 80 CNY/t threshold applies to the capture stage only. Including CO₂ transport and storage would raise the full-chain CCUS cost by approximately 30–80 CNY/t CO₂, depending on transport distance and storage site conditions, shifting the economic viability threshold to around 120–150 CNY/t CO₂. This range aligns with full-chain CCUS cost assessments reported for China's coal chemical clusters [51,52]. Nevertheless, the proximity of major bases (e.g., Ordos, Ningdong) to Ordos Basin storage sites could partially offset transport costs. We therefore recommend a progressive carbon pricing trajectory complemented by targeted CCUS subsidies, aiming for the carbon price to effectively break through this key threshold around 2030, while also considering differentiated support that accounts for full-chain costs and regional storage advantages.

4.2. Trade-Offs and Synergies

The Shapley value analysis reveals a significant trade-off between the short and long term. Comprehensive resource utilization technology R (gasification slag and fly ash comprehensive utilization) contributes the most in the near term (2025), but its marginal benefit declines year by year, reflecting the characteristic that end-of-pipe treatment and resource recovery pathways tend to deliver early results. Although the marginal contributions of green hydrogen substitution technology S1 and CCUS and green hydrogen coupling technology S2 are extremely low in 2025, with Shapley values approaching zero, their long-term contributions rise steadily and become absolutely dominant by 2050. This finding confirms that the model of reducing pollution through carbon mitigation is more aligned with long-term emission reduction needs [54–56]. The LMDI decomposition results offer further support at the driver level, showing that the contribution rate of the technology reduction effect rose from 21% to 47% during 2030 to 2050, surpassing the scale effect to become the largest emission reduction driver. It should be noted that although end-of-pipe technologies such as CCUS can achieve significant CO₂ emission reductions, they may entail increased energy consumption and operating costs [57,58], whereas clean feedstock substitution pathways like green hydrogen, despite higher initial costs, yield more pronounced long-term synergistic benefits [59–61].

4.3. Policy Recommendations

Based on the findings that policy and technology uncertainties dominate the presence of threshold effects for carbon price and green hydrogen cost, and the identified short-term versus long-term trade-offs in technology portfolios, this study recommends reinforcing policy design in the areas of a dynamic response mechanism, risk-hedging strategies, regionally differentiated deployment, and watershed collaborative governance. At the policy design level, a dynamic threshold response mechanism should be established to automatically activate dedicated CCUS subsidies once the carbon price exceeds 80 CNY per tonne and to accelerate the commercialization of green hydrogen as its cost falls below 6.8 CNY per kilogram, thereby creating an effective linkage between price signals and technology deployment. To avoid the inherent uncertainty of relying on a single technology pathway, a technology portfolio fund should be set up to guide enterprises toward risk-hedging routes that integrate gasification slag utilization with CCUS and renewable energy. Spatially, differentiated deployment strategies should be adopted according to regional resource endowments. Regions abundant in wind and solar resources, including Ningxia, Qinghai, Inner Mongolia, and Gansu, should prioritize direct green electricity supply and the coupling of CCUS with green hydrogen, whereas traditional industrial clusters in Shanxi, Shandong, and Henan should emphasize resource comprehensive utilization and energy-saving retrofits in the near term while gradually incorporating novel low-carbon technologies. The effective implementation of these measures also depends on watershed-scale collaborative governance, which encompasses establishing a cross-provincial joint monitoring platform for pollutants and carbon emissions [62,63], implementing a synergistic water, carbon, and energy management mechanism [64,65], and taking the lead in introducing a full-life cycle carbon labeling system for coal chemical products in the Yellow River Basin [66].

4.4. Limitations and Future Research

This study has several limitations. Carbon emission data for some provinces prior to 2021 are incomplete, and future efforts should strengthen the retroactive compilation and verification of historical data. The model has not yet fully incorporated the uncertainty transmission effects along the upstream and downstream supply chain, such as the impact of coal price fluctuations on the competitiveness of coal chemical products. Market penetration pathways for emerging coal chemical products, including coal-to-fine chemicals, have not been integrated into the model framework, which may affect the accurate assessment of long-term emission reduction potential. Moreover, the system dynamics model employed is a simplified version and does not fully capture the complex nonlinear relationships inherent in real production systems. Future research could proceed along several directions: introducing artificial intelligence methods to predict the impacts of extreme climate events on the industry, developing a life cycle supply chain uncertainty analysis framework, and conducting empirical validation studies at the enterprise level.

5. Conclusions

This study constructed a multi-level uncertainty conduction model to systematically quantify the impacts of policy, technology, market, and ecological uncertainties on the synergistic pathways of pollution reduction and carbon mitigation in the coal chemical industry of the Yellow River Basin. The results indicate that policy and technology uncertainties are the dominant factors constraining synergistic benefits, with variance contribution rates of 35% and 28%, respectively. A carbon price of 80 CNY per tonne and a green hydrogen cost of 6.8 CNY per kilogram constitute two critical thresholds, triggering a structural leap in CCUS economic viability and the large-scale deployment of green hydrogen substitution,

respectively, and revealing the nonlinear nature of synergistic governance dominated by nested multiple thresholds. The dynamic threshold response mechanism and technology portfolio hedging strategy we propose are expected to increase synergistic benefits by 22% to 35%, suggesting that proactively managing uncertainty itself can constitute a significant emission reduction gain. In terms of technology pathways, comprehensive resource utilization, CCUS coupled with green hydrogen, green hydrogen substitution, and direct green electricity supply exhibit a sequential, cascading temporal structure, requiring policy design to accommodate the integration of technologies at different maturity levels. Spatially, regions rich in wind and solar resources and traditional industrial agglomerations form a complementary pattern in emission reduction timelines and technology choices. We recommend establishing a life cycle carbon labeling system for coal chemical products in the Yellow River Basin, thereby promoting a shift in collaborative watershed governance from an administrative-driven to a standard-driven approach.

Despite these contributions, this study has several limitations, including incomplete historical data for some provinces, failure to address supply chain uncertainty and emerging product pathways, and simplifications in the system dynamics model. Future research will address these through AI-based extreme event prediction, life cycle supply chain analysis, and enterprise-level empirical validation.

Supplementary Materials: The following supporting information can be downloaded at <https://www.mdpi.com/article/10.3390/app16136747/s1>, Table S1: Coal chemical production in the Yellow River Basin (Mt) [1–4]; Table S2: Key parameters and reference sources [5,23–25,67–69]; Table S3: Carbon emission factors for different production processes [25,69–73]; Table S4: Pollutant emission factors in the production process of coal chemical products; Table S5: Emission reduction scenario development for the coal chemical industry in the Yellow River Basin [74–77]; Table S6: Costs of different emission reduction technologies [68,77–87]; Table S7: Probability distribution parameters; Table S8: Key parameters for the Sobol’ analysis; Table S9: Comparison of multi-level sensitivity analysis methods; Table S10: Emission reduction technology inventory for the Shapley value analysis; Table S11: Grouping of emission reduction technologies for Shapley value analysis; Table S12: Shapley values for different years; Table S13: Logistic S-curve diffusion parameters; Table S14: Technology penetration rates across scenarios.

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