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

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1. Data and Sources

Table S1 Coal chemical production in the Yellow River Basin (Mt)

	2023	2030	2050
Coal to coke	274	228	115
Coal to synthetic ammonia	24	21	26
Coal to methanol	51	31	34
Coal to ethylene glycol	8	10	21
Coal to natural gas	3	13	59
Direct coal to oil production	1	1	2
Coal indirect oil production	9	13	25
Coal to olefin	12	25	35

Traditional coal chemical production data for 2023 were sourced from statistical yearbooks. Production figures for 2030 and 2050 were derived from literature surveys [1-4], all of which have been cited in the main text. Modern coal chemical product output data were obtained from a survey of modern coal chemical projects in the Yellow River Basin.

Table S2 Key parameters and reference sources

Coal chemical products	Carbon emission factor (tCO_2 t)[5]				Energy consumption per unit of coal chemical products			
	Chemical processes	Fuel combustion	Upstream processes	Total	Fuel coal (t/t)[25, 67, 68]	Electricity (MWh/t)[23, 24, 69]	Heat (GJ/t)[23]	Raw materials (t/t)[5]
Direct coal to oil production	2.93	1.09	1.22	5.24 (4.23-6.23)	0.55	0	0	3.9
Coal indirect oil production	4.93	2.08	1.92	8.93 (8.12-9.83)	1.04	1.1	0	3.7
Coal to natural gas	4.87	1.51	1.25	7.62 (7.10-8.17)	0.76	0.25	0.54	3.1
Coal to olefin	6.58	2.38	3.29	12.7 (12.7-13.7)	1.2	2.69	0	5
Coal to ethylene glycol	4.19	5.94	1.69	12.0 (11.0-13.0)	2.98	0.62	0	2.7
Coal to coke	0.12	0.033	0.47	0.62 (0.60-0.63)	0.017	0.057	0.25	1.4
Coal to synthetic ammonia	3.14	0.78	0.96	4.89 (4.68-5.11)	0.39	0.85	0	1.3
Coal to methanol	2.55	1.56	0.71	4.82 (4.55-5.07)	0.78	0.28	0	1.4

Table S3 Carbon emission factors for different production processes

	Carbon emission factor	Value	Unit	Reference
In-situ	Coal combustion	1.99	$kgCO_2eq/kg$	[25]
	Natural gas combustion	2.16	$kgCO_2eq/m^3$	[25]
Life cycle	Fuel coal production	0.180	$kgCO_2eq/kg$	[70]
	Feedstock coal production	0.288	$kgCO_2eq/kg$	
	Fuel natural gas production	0.279	$kgCO_2eq/m^3$	
	Outsourced heat supply	0.126	$kgCO_2eq/MJ$	
	Photovoltaic power generation	0.0362	tCO_2eq/MWh	[71]
	Onshore wind power	0.0199	tCO_2eq/MWh	[72]
	Grid electricity (2022)	0.5366	tCO_2eq/MWh	[69]
	Grid electricity (2030 renewable energy mix)	0.400	tCO_2eq/MWh	[73]
	Grid electricity (2050 renewable energy mix)	0.114	tCO_2eq/MWh	

The life-cycle pollutant emission factors and removal efficiencies for the coal chemical industry were adopted from the average values in the Industrial Source Production and Discharge Accounting Methods and Coefficients Manual (2017). The specific values used are listed below.

Table S4 Pollutant emission factors in the production process of coal chemical products

Products	Pollutant	Unit	Generation factors	Average removal rate (%)	Pollutant equivalent
Coal to coke	Ammonia (NH_3)	kg/t-product	0.002	95	9.09
	Ammonia nitrogen (NH_3-N)	g/t-product	104.65	95	0.8
	Nitrogen oxides (NO_x)	kg/t-product	0.405	85	0.95
	Sulfur dioxide (SO_2)	kg/t-product	0.418	90	0.95
	Chemical oxygen demand (COD)	kg/t-product	0.875	97	1
	Volatile phenols (VP)	g/t-product	225	99	0.08
	Volatile organic compounds (VOCs)	kg/t-product	1.016	33.5	0.95
	Particulate matter (PM)	kg/t-product	0.953	99	2.36
	Cyanide (CN)	g/t-product	4.75	95	0.05
	Petroleum hydrocarbons (PP)	g/t-product	105.2	99	0.1
	Total nitrogen (T-N)	g/t-product	158.5	96	0.8
	Total phosphorus (T-P)	g/t-product	17.2	96	0.25
Coal to synthetic	Ammonia nitrogen (NH_3-N)	kg/t-product	0.282	74.40	0.8
	Nitrogen oxides (NO_x)	kg/t-product	0.705	53.00	0.95

ammonia	Sulfur dioxide (SO_2)	kg/t-product	0.554	82.75	0.95
	Chemical oxygen demand (COD)	kg/t-product	2.298	86.20	1
	Volatile phenols (VP)	kg/t-product	0.001	68.33	0.08
	Volatile organic compounds (VOCs)	kg/t-product	0.11	78.00	0.95
	Particulate matter (PM)	kg/t-product	2.165	94.00	2.36
	Cyanide (CN)	kg/t-product	0.001	67.67	0.05
	Petroleum hydrocarbons (PP)	kg/t-product	0.019	73.00	0.1
	Total nitrogen (T-N)	kg/t-product	0.468	75.40	0.8
	Total phosphorus (T-P)	kg/t-product	0.00362	69.00	0.25
Coal to methanol	Ammonia nitrogen (NH_3-N)	kg/t-product	0.00188	90	0.8
	Chemical oxygen demand (COD)	kg/t-product	0.116	98	1
	Total nitrogen (T-N)	kg/t-product	0.00152	90	0.8
Coal to natural gas	Ammonia nitrogen (NH_3-N)	kg/t-feedstock	2.080	93	0.8
	Sulfur dioxide (SO_2)	kg/t-feedstock	0.78	97.67	0.95
	Chemical oxygen demand (COD)	kg/t-feedstock	5.688	93	1
	Volatile phenols (VP)	kg/t-feedstock	1.925	79.5	0.08
	Volatile organic compounds (VOCs)	kg/t-feedstock	0.0735	70	0.95
	Particulate matter (PM)	kg/t-feedstock	1.140	99	2.36
	Cyanide (CN)	kg/t-feedstock	0.015	73	0.05
	Petroleum hydrocarbons (PP)	kg/t-feedstock	0.420	92	0.1
	Total nitrogen (T-N)	kg/t-feedstock	1.685	93.67	0.8
coal to oil	Chemical oxygen demand (COD)	kg/t-product	8.244	72.5	1
	Petroleum hydrocarbons (PP)	kg/t-product	0.088	80.5	0.1
Coal to olefin	Nitrogen oxides (NO_x)	kg/t-product	0.014	40	0.95
	Chemical oxygen demand (COD)	kg/t-product	0.45	90	1
	Particulate matter (PM)	kg/t-product	0.071	99	2.36
Coal to ethylene glycol	Ammonia nitrogen (NH_3-N)	kg/t-product	0.037	20	0.8
	Chemical oxygen demand (COD)	kg/t-product	1.5	80	1
	Petroleum hydrocarbons (PP)	kg/t-product	0.0000034	70	0.1
	Total nitrogen (T-N)	kg/t-product	0.03	90	0.8
Coal	Ammonia nitrogen (NH_3-N)	g/t-coal	1.41	85	0.8
	Chemical oxygen demand (COD)	g/t-coal	33.16	87.5	1
	Petroleum hydrocarbons (PP)	g/t-coal	2.31	90	0.1
Electricity	Ammonia nitrogen (NH_3-N)	g/t-feedstock	17.28	84.01	0.8

and heat	Chemical oxygen demand (COD)	g/t-feedstock	83.75	65.69	1
	Nitrogen oxides (NO_x)	g/t-feedstock	2.39	72.04	0.95
	Sulfur dioxide (SO_2)	g/t-feedstock	18.61	93.61	0.95
	Particulate matter (PM)	g/t-feedstock	193.145	99.92	2.36

Table S5 Emission reduction scenario development for the coal chemical industry in the Yellow River Basin [74-77]

Emission reduction measures		2023	Baseline scenario			Policy scenario			Strengthened scenario		
First level	Second level		2025	2030	2050	2025	2030	2050	2025	2030	2050
Raw material structure adjustment	green hydrogen substitution (S1)	0	0	5	25	1	10	50	3	15	75
	CCUS+Green Hydrogen Coupled Methanol Production Technology (S2)	0	0	5	25	1	10	50	3	15	75
Energy structure adjustment	Electrification transformation or centralized energy supply (ES1)	0	0	5	25	1	10	50	3	15	75
	Green Power Direct Supply (ES2)	0	0	5	25	1	10	50	3	15	75
Upgrading energy-saving technology	Energy-saving coating technology for high-temperature industrial kilns (T1)	3	5	25	50	10	50	95	20	75	100
	Intelligent Load Adjustment of Coal fired Boilers Towards Zero Ash Accumulation and Zero Condensation Depth Energy saving Technology (T2)	35	50	80	100	55	90	100	60	100	100
	Three effect solvent recovery energy-saving distillation technology (T3)	54	60	80	100	65	90	100	70	100	100
	Modular cascade regenerative clean coal gasification technology (T4)	26	30	40	95	35	50	100	45	75	100
	Energy saving technology for park type new energy microgrid (T5)	11	15	25	80	20	35	90	30	55	100
	Low grade waste heat recovery and utilization technology for industrial coal-fired unit flue gas (T6)	8	10	15	60	15	25	90	20	35	100
	Energy saving technology of self	2	3	5	20	5	10	50	7	15	60

	regenerative distillation (T7)										
	Horizontal oil cooled permanent magnet governor (T8)	26	30	40	80	35	50	90	45	75	100
End of pipe technology transformation	CCUS technology (ET)	0	0	5	25	1	10	50	3	15	75
Comprehensive utilization technology	Gasification slag and fly ash for resource utilization (R)	52	55	60	80	58	65	90	60	65	90

Table S6 Costs of different emission reduction technologies

Technology	Year	Cost	Reference
Hydrogen production by wind-based electrolysis	2020	28.52 CNY/kg H_2	[78, 79]
Hydrogen production by solar-powered electrolysis	2020	25.71 CNY/kg H_2	[78, 80-82]
Hydrogen production by renewable energy electrolysis	2020	29.1 CNY/kg H_2	[68, 83]
	2030	15 CNY/kg H_2	
	2050	6.5 CNY/kg H_2	
	2060	5.2 CNY/kg H_2	
Electricity	2025	0.54 CNY/kWh	Average values were calculated based on the electricity price schedules for industrial and commercial users from proxy power purchases by electric power companies in the nine provinces of the basin.
	2030	0.47 CNY/kWh	IRENA
	2050	0.37 CNY/kWh	IEA，IRENA
Coal	2025	750 CNY/吨	China National Coal Association
CCUS	2025	210 CNY/吨	[84-87]
	2030	150 CNY/吨	
	2050	100 CNY/吨	
Comprehensive utilization technology of gasification slag and fly ash	2025	-250 CNY/吨	[77]

2. Uncertainty Analysis Methodology

2.1 Synergistic Effect Assessment Framework

2.1.1 Accounting for carbon and pollutant emissions

We collected the 2020 carbon emission factors to estimate emissions from China's coal chemical industry, including those from chemical reactions and fuel combustion. To facilitate a comprehensive cost-benefit comparison with carbon emissions, we aggregate multiple pollutants into a unified 'pollutant emission equivalent'. This aggregation was based on pollution equivalent values stipulated in the Environmental Protection Tax Law of the People's Republic of China (revised in 2018). Using provincial production data for coal chemical products and projects along with the corresponding emission factors, we calculated the carbon and pollutant emissions for the baseline scenarios in 2023, 2030, and 2050.

$$P_c = \sum_i \sum C_i \times a_{ix} \tag{1}$$

$$P_{pj} = \sum_i \sum C_i \times b_{ijx} \tag{2}$$

$$P_p = \sum_j \left(P_{pj} \times D_{pj} \right) \tag{3}$$

Where P_{pj} is the emission of the j-th pollutant, b_{ijx} is the emission coefficient of the j-th pollutant for the i-th coal chemical product at production stage x, P_p is the pollutant emission equivalent, and D_{pj} is the emission equivalent coefficient of the j-th pollutant.

2.1.2 Determination of weights for the composite synergistic benefit index

A questionnaire survey was administered to ten experts specializing in coal chemical industry and environmental economics. The analytic hierarchy process (AHP) was combined with expert scoring to derive the indicator weights. The consistency ratio (CR) of the judgment matrix was 0.021 (<0.1), confirming satisfactory consistency. The final weights assigned were carbon emission reduction potential $w_c = 0.4$, pollutant reduction $w_p = 0.3$, and cost-effectiveness $w_{cost} = 0.3$. A sensitivity analysis examined the impact of varying each weight within ±10% of its base value (e.g., $w_c \in [0.36, 0.44]$) on the assessment outcomes. The Kendall τ correlation coefficient between the resulting synergistic benefit rankings and the original ranking exceeded 0.92, demonstrating strong robustness of the ranking results.

2.2 Probability distributions of key uncertainty parameters

The probability distributions of the key uncertainty parameters are presented in Table S7, and the rationale for selecting each distribution form is described below.

For the carbon price distribution, a bounded distribution was adopted to reflect the upper and lower limits imposed by policy regulation. The lower bound was set at 30 CNY/t, corresponding to the carbon market floor price, the upper bound at approximately 300 CNY/t, referencing international carbon prices, and the mode at 80 CNY/t, which corresponds to the economic viability threshold for CCUS.

Green hydrogen cost follows a technology learning curve, characterized by a trajectory of high initial cost, rapid decline, and gradual convergence. A log-normal distribution was chosen because it ensures the cost variable remains non-negative while reasonably reproducing this dynamic process.

Multiple engineering cases have shown that CCUS technology cost fluctuates symmetrically around its mean, and therefore a normal distribution was employed to characterize it.

Water resource availability in the Yellow River Basin exhibits right-skewed and non-negative statistical characteristics, and a Gamma distribution was selected to match the typical distribution form of such hydrological variables.

The energy efficiency decay rate is a bounded variable within the interval [0,1]. The Beta distribution was adopted due to its flexibility in effectively describing the typical pattern of equipment performance degradation.

Table S7 Probability distribution parameters

Parameter ID	Parameter name	DPSIR dimension	Distribution type	Distribution parameters	Data source/basis
U01	Carbon price (CNY/t)	Policy	Triangular	min=30, mode=80, max=300	Historical prices in the national carbon market (2021–2023) and international carbon price benchmarking
U02	Policy enforcement intensity coefficient	Policy	Uniform	[0.8, 1.2]	Literature survey on policy implementation deviation
U03	Frequency of emission standard tightening (times per 5 years)	Policy	Poisson	$\lambda=2$	Historical frequency of emission standard revisions during 2010–2023
U04	CCUS cost (CNY/t CO_2)	Technology	Normal	$\mu=70$, $\sigma=15$	IEA and GCCSI technology report (2023)
U05	Green hydrogen cost (CNY/kg)	Technology	Log-normal	$\mu=\ln(15)$, $\sigma=0.4$	White paper of the China Hydrogen Alliance and learning curve projection
U06	Energy efficiency decay rate	Technology	Beta	$\alpha=2$, $\beta=5$	Engineering practice experience (equipment aging patterns)
U07	Technology penetration rate fluctuation coefficient	Technology	Uniform	[0.8, 1.2]	Statistics on achievement rates of historical promotion plans
U08	Coal price volatility	Market	Normal	$\mu=0$, $\sigma=0.2$	Historical volatility of steam coal price at Qinhuangdao Port (2011–2023)
U09	Product demand elasticity	Market	Uniform	[-0.5, 0.5]	Literature review on demand elasticities of coal chemical products
U10	Electricity carbon emission factor (2023 baseline)	Market	Normal	$\mu=0.581$, $\sigma=0.05$	Announcement of grid emission factors by the Ministry of Ecology and Environment
U11	Water resource availability coefficient	Ecology	Gamma	$k=5$, $\theta=0.2$	Hydrological statistics of the Yellow River Basin (2000–2023)
U12	Frequency of extreme climate events (times per 5 years)	Ecology	Poisson	$\lambda=1$	Disaster statistical bulletins of the China Meteorological Administration (2000–2023)

2.3 Sobol' global sensitivity analysis setup and comparison of multi-level methods

（1）Key parameters for the Sobol' global sensitivity analysis

The key parameters involved in the Sobol' global sensitivity analysis are listed in Table S8. Specifically, parameter P11 was assigned the relative standard deviation of the carbon emission accounting factor to characterize the uncertainty in emission accounting. Parameter P6 was set as a variation range relative to its baseline value, taken as 100%.

Table S8 Key parameters for the Sobol' analysis

Parameter ID	Parameter name	Unit	Lower bound	Upper bound
P1	Carbon price	CNY/t	50	300
P2	CCUS technology penetration rate	%	0	75
P3	Green hydrogen cost	CNY/kg	5	30
P4	Green electricity penetration rate	%	0	75
P5	Comprehensive resource utilization penetration rate	%	50	90
P6	Product structure adjustment range	%	−60	200
P7	Coal price fluctuation	dimensionless	−0.3	0.3
P8	Electricity carbon emission factor	t CO_2/MWh	0.4	0.7
P9	Water resource availability coefficient	dimensionless	0.3	1.5
P10	VOCs control policy intensity	dimensionless	0.5	2
P11	Carbon emission factor uncertainty	dimensionless	0.05	0.3
P12	Energy efficiency decay rate	dimensionless	0.05	0.4
P13	Coal-to-olefins production growth	10^4 t	100	800
P14	Coal-to-natural gas production growth	10^4 t	50	2000
P15	Industrial water price	CNY/t	1.5	4.5

(2) Saltelli sampling scheme

The Sobol' global sensitivity analysis was designed according to the Saltelli method. The base sample size was set to N = 1,024 (2^{10}), which satisfies the basic requirement of the method for sample size, and the parameter dimensionality was D = 15. Two independent base sampling matrices, A and B, each of size N × D, were first generated. Subsequently, each column i of matrix A was replaced by the corresponding column of matrix B to construct 15 matrices $A_B^{(i)}$. The number of model evaluations per objective thus equals N × (D + 2) = 1,024 × 17 ≈ 17,408. Given that the study involves three objective functions, the total number of evaluations reaches 17,408 × 3 = 52,224. Samples were generated using low-discrepancy Sobol sequences, which achieve better uniformity of coverage in the parameter space compared with conventional pseudo-random sequences. For the 17,408 output samples obtained from the single-objective analysis, 100 Bootstrap resamples were performed, and the 95% confidence intervals of the first-order sensitivity index S1 and the total-effect index S_T were calculated.

（3）Sobol sensitivity index calculation

First-order index S_1：

$$S_{1i} \approx \frac{\frac{1}{N}\sum_{j=1}^{N} f(B)_j \left[f\left(A_B^{(i)}\right)_j - f(A)_j \right]}{V(Y)} \tag{4}$$

Total-effect index S_T:

$$S_{Ti} \approx \frac{\frac{1}{2N}\sum_{j=1}^{N}\left[f(A)_j - f\left(A_B^{(i)}\right)_j\right]^2}{V(Y)} \quad (5)$$

Total variance V(Y):

$$V(Y) = \frac{1}{N}\sum_{j=1}^{N} f(A)_j^2 - \left[\frac{1}{N}\sum_{j=1}^{N} f(A)_j\right]^2 \quad (6)$$

Where $f(A)_j$, $f(B)_j$, and $f(A_B^{(i)})_j$ denote the model outputs, specifically carbon emission reduction, pollutant reduction, and cost-effectiveness, when the j-th row of matrices A, B, and $A_B^{(i)}$ is used as input, and N is the sample size. A convergence test was performed to examine the influence of sample size on index stability. The total-effect index S_T was computed for base sample sizes of N=512, 1024, and 2048. The Kendall τ correlation coefficient between the S_T rankings obtained with N=1024 and N=2048 exceeded 0.96, indicating that N=1024 is sufficient to ensure convergence of the sensitivity indices.

(4) Comparison of the multi-level sensitivity analysis methodological framework

Table S9 Comparison of multi-level sensitivity analysis methods

Method	OAT local sensitivity	Sobol global sensitivity	Shapley value analysis	MC variance decomposition
Type	Local	Global	Game theory	Statistical
Analysis object	Single parameter	15 parameters	14 technologies	4 dimensions
Core output	Parameter variation versus output variation curve	S_1, S_T indices	Marginal contribution φ(i)	Variance contribution rate %
Computational complexity	Low (k×n)	High (N×(D+2))	Medium (2^{14}=16,384 combinations)	High (10,000 simulations)
Advantages	Intuitive and easy to understand, fast computation	Handles nonlinear interactions, model-assumption free	Fair allocation, considers cooperative games	Macro-level ranking
Limitations	Ignores interaction effects	Computationally intensive	Number of combinations grows exponentially with technology count	Rough (does not decompose contributions of specific parameters within a dimension)
Application scenarios	Preliminary screening of key parameters	Identification of key driving factors	Allocation of technology contributions	Macro judgment of dimension importance

2.4 Shapley value analysis of technology contributions

(1) The emission reduction technology inventory is presented in Table S10.

Table S10 Emission reduction technology inventory for the Shapley value analysis

Technical code	Technical name	Technical classification	2023 penetration rate	Main application subsectors
S1	Green hydrogen substitution (coal gasification to hydrogen replaced by	Feedstock structure	0%	Synthetic ammonia, methanol,

	renewable energy electrolysis to hydrogen)	substitution		coal-to-liquids
S2	CCUS and green hydrogen coupling to methanol	Feedstock structure substitution	0%	Methanol
E1	Electrification retrofitting / centralized energy supply	Energy structure optimization	0%	Industry-wide
E2	Direct green electricity supply (wind/solar)	Energy structure optimization	0%	Industry-wide
T1	High-temperature industrial furnace infrared energy-saving coating	Energy-saving technology	3%	Coke, synthetic ammonia
T2	Coal-fired boiler intelligent load regulation energy-saving technology	Energy-saving technology	35%	Coke, synthetic ammonia, methanol
T3	Triple-effect solvent recovery energy-saving distillation technology	Energy-saving technology	54%	Methanol, ethylene glycol
T4	Modular cascade regenerative gasification technology (MCREG)	Energy-saving technology	26%	Synthetic ammonia, methanol
T5	Park-level new energy microgrid energy-saving technology	Energy-saving technology	11%	Industry-wide
T6	Flue gas waste heat recovery and utilization for industrial coal-fired units	Energy-saving technology	8%	Industry-wide
T7	Self-heat recuperative distillation energy-saving technology	Energy-saving technology	2%	Ethylene glycol, olefins
T8	Horizontal oil-cooled permanent magnet speed governor	Energy-saving technology	26%	Industry-wide
End	CCUS technology (post-combustion chemical absorption)	End-of-pipe treatment	0%	Industry-wide
R	Gasification slag and fly ash comprehensive utilization technology	Comprehensive resource utilization	52%	Coke, synthetic ammonia, methanol

(2) Technology grouping and group contribution calculation

The emission reduction technologies were classified into five groups. The Shapley value for each group was obtained by summing the Shapley values of the technologies within that group.

Table S11 Grouping of emission reduction technologies for Shapley value analysis

Group	Technologies included	Group type
Feedstock structure group	S1, S2	Disruptive low-carbon technologies
Energy structure group	E1, E2	Disruptive low-carbon technologies
Energy-saving technology group	T1 to T8	Incremental low-carbon technologies
End-of-pipe treatment group	End	Compensatory low-carbon technology
Comprehensive resource utilization group	R	Circular economy technology

(3) Synergy factor sensitivity analysis

A synergy factor $(1+\beta\cdot(|S|-1))$ was introduced into the characteristic function $v(S) = \omega_c C_S + \omega_p P_S + \omega_{cost}\Delta C_S$, where β is the synergy gain coefficient. The value of β was determined based on experiments with 12 technology combinations. By comparing the sum of effects when technologies are implemented independently with the measured effects after combined implementation, β was found to range from 0.03 to 0.08, with a median of 0.05; hence, β = 0.05 was adopted for the baseline calculation. To test the robustness of the ranking results, Shapley values were recalculated with β = 0.03 and β = 0.07. The Kendall τ correlation coefficients between the resulting technology contribution rankings and the baseline ranking both exceeded 0.94, indicating that the Shapley value ranking is insensitive to variations in the synergy factor and the conclusions are reliable.

(4) Complete Shapley value data for 2025, 2030, and 2050

Table S12 Shapley values for different years

Technical ID	2025 Shapley value	Contribution rank	2030 Shapley value	Contribution rank	2050 Shapley value	Contribution rank
S1	0.003	14	0.042	9	0.187	1
S2	0.005	13	0.058	6	0.175	2
E1	0.008	12	0.035	10	0.082	6
E2	0.009	11	0.051	7	0.125	3
T1	0.035	7	0.032	11	0.018	13
T2	0.068	3	0.062	5	0.024	11
T3	0.052	5	0.048	8	0.021	12
T4	0.042	6	0.065	4	0.035	10
T5	0.018	9	0.028	12	0.045	8
T6	0.022	8	0.025	13	0.012	14
T7	0.011	10	0.018	14	0.038	9
T8	0.058	4	0.068	3	0.052	7
End	0.006	12	0.078	2	0.098	5
R	0.125	1	0.112	1	0.103	4

The Shapley value decomposition results indicate that in 2025, the comprehensive resource utilization technology (R) achieved a Shapley value of 0.125, markedly higher than the other technologies, suggesting that end-of-pipe resource recovery represents the most cost-effective emission reduction pathway in the near term. In 2030, although technology R still ranked first, its lead had narrowed; the CCUS end-of-pipe treatment technology (End) rose to second place, and direct green electricity supply (E2) entered the top seven, reflecting the emerging role of novel low-carbon technologies. By 2050, green hydrogen substitution (S1) and CCUS–green hydrogen coupling (S2) had jumped to the top two positions, jointly contributing approximately 36% and assuming a dominant role; technology R fell to fourth place but still retained a notable contribution.

2.5 System dynamics model and MINLP optimization model

2.5.1 Equations and parameters of the system dynamics model

(1) Industrial development subsystem equations

Dynamics of traditional coal chemical capacity (CAP_{trad}):

$$\frac{dCAP_{trad}}{dt}=-r_{decay}\times CAP_{trad} \tag{7}$$

Where, r_{decay} denotes the decay rate, with values of 2% under BAU, 3% under ESP, 2.5% under TBS, and 3.5% under CUS.

The dynamics of modern coal chemical capacity (CAP_{modern}):

$$\frac{dCAP_{modern}}{dt}=r_{growth}\times CAP_{modern}\times(1-\frac{CAP_{modern}}{CAP_{sat}}) \tag{8}$$

Where, r_{growth} represents the growth rate, set to 3% for BAU, 4% for ESP, 5% for TBS, and 2% for CUS; CAP_{sat} denotes the market saturation capacity, and the maximum modern coal chemical capacity is taken as 200 million tonnes of standard coal equivalent per year in this study.

Total capacity:

$$CAP_{total}=CAP_{trad}+CAP_{modern} \tag{9}$$

(2) Pollution emission subsystem

The emission of the k-th pollutant ($E_{pol,k}$):

$$E_{pol,k}=CAP_{trad}\times EF_{trad,k}+CAP_{modern}\times EF_{modern,k}\times(1-T_k) \tag{10}$$

$$T_k=1-\prod_{j=1}^{14}\left(1-P_j\times\eta_{jk}\right) \tag{11}$$

Where, $EF_{trad,k}$ and $EF_{modern,k}$ denote the emission factors for the k-th pollutant from traditional and modern capacity, respectively; T_k is the technology abatement efficiency. P_j represents the penetration rate of technology j, and η_{jk} is the removal efficiency of technology j for pollutant k.

Total pollutant equivalent (P_{eq}):

$$P_{eq}=\sum_{k}^{12}\frac{E_{pol,k}}{E_k^{ref}} \tag{12}$$

Where, E_k^{ref} denotes the pollution equivalent of pollutant k.

(3) Carbon cycle subsystem equations

Total carbon emissions (E_{CO2}) comprise four components: process emissions from feedstock consumption ($E_{feedstock}$), direct emissions from fuel combustion (E_{fuel}), indirect emissions from purchased electricity and heat ($E_{electricity}$), and carbon removal captured and stored via CCUS technology (E_{CCUS}).

$$E_{CO2}=E_{feedstock}+E_{fuel}+E_{electricity}-E_{CCUS} \tag{13}$$

$$E_{feedstock}=CAP_{total}\times a\times EF_{process}\times(1-P_{S1}\times\eta_{S1}) \tag{14}$$

$$E_{fuel}=CAP_{total}\times b\times EF_{fuel}\times(1-P_{E2}\times\eta_{E2}) \tag{15}$$

$$E_{electricity}=EC\times EF_{grid}\times(1-P_{E1}\times\eta_{E1}-P_{E2}\times\eta_{E2}) \tag{16}$$

$$E_{CCUS}=E_{CO2}\times P_{End}\times\eta_{capture} \tag{17}$$

Where, a is the capacity utilization rate. $EF_{process}$ represents the process emission factor. PS1 is the penetration rate of green hydrogen substitution, and η_{S1} its emission reduction efficiency. B denotes the fuel consumption coefficient, and EF_{fuel} the fuel emission factor. P_{E2} is the penetration rate of direct green electricity supply technology, with η_{E2} as its reduction efficiency. EC is the

total purchased electricity consumption. EF_{grid} stands for the regional grid carbon emission factor. P_{E1} is the penetration rate of electrification retrofitting technology, and η_{E1} its reduction efficiency. P_{End} indicates the penetration rate of CCUS technology, and $\eta_{capture}$ the CO_2 capture efficiency.

Autonomous decline of carbon emission intensity ($EF_{all}(t)$):

$$EF_{all}(t)=EF_{all}(t\text{-}1)\times(1\text{-}r_{AEEI}) \tag{18}$$

Where, t denotes the year, and r_{AEEI} represents the autonomous energy efficiency improvement rate, set at 2% under BAU, 2.5% under ESP, 3% under TBS, and 2%–3% under CUS.

(4) Policy regulation subsystem equations

Carbon price dynamics:

$$P_{carbon}(t)=P_{carbon}(2023)\times(1+r_{carbon})^{t\text{-}2023} \tag{19}$$

Where, $P_{carbon}(t)$ denotes the carbon price in year t, $P_{carbon}(2023)$ is the base-year carbon price, and r_{carbon} represents the annual carbon price growth rate, set at 3% for BAU, 5% for ESP, 4% for TBS, and 6% for CUS.

Technology penetration follows a logistic S-curve:

$$P_j(t)=P_{j,base}+\frac{P_{j,max}\text{-}P_{j,base}}{1+exp(\text{-}k_j\times(t\text{-}t_{inf,j}))} \tag{20}$$

Where, $P_j(t)$ denotes the penetration rate of technology j in year t. $P_{j,base}$ is the baseline penetration rate, defined as the actual deployment level in 2023. $P_{j,max}$ is the saturation penetration rate, k_j is the diffusion rate parameter, and $t_{inf,j}$ is the inflection year.

Technology coupling acceleration factor:

$$k_j^{'}=k_j\times(1+r_{jl}\times P_l) \tag{21}$$

Where k_j' denotes the modified diffusion rate of technology j when deployed synergistically with technology l. γ_{jl} is the coupling acceleration coefficient, characterizing the enhancement effect of technology l deployment on the diffusion rate of technology j. P_l represents the current penetration rate of technology l deployed in synergy with technology j.

(5) Logistic S-curve diffusion parameter table

Table S13 Logistic S-curve diffusion parameters

Technology ID	Technology maturity category	k_j (standard diffusion rate)	t_{inf} (BAU)	t_{inf} (ESP)	t_{inf} (TBS)	Baseline penetration rate P_{base}	Saturation penetration rate P_{max}
S1	Frontier technology	0.18	2040	2035	2030	0%	25–75%*
S2	Frontier technology	0.18	2040	2035	2030	0%	25–75%*
E1	Emerging technology	0.22	2038	2033	2028	0%	25–75%*
E2	Emerging technology	0.22	2038	2033	2028	0%	25–75%*
T1	Near-term mature	0.4	2032	2028	2025	3%	50–100%*
T2	Near-term mature	0.45	2030	2026	2025	35%	80–100%*
T3	Near-term mature	0.45	2028	2025	2025	54%	90–100%*
T4	Near-term mature	0.35	2032	2028	2026	26%	95–100%*
T5	Emerging technology	0.25	2036	2032	2028	11%	80–100%*
T6	Near-term mature	0.3	2034	2030	2028	8%	60–100%*
T7	Near-term mature	0.28	2038	2035	2032	2%	20–60%*

T8	Near-term mature	0.35	2034	2030	2028	26%	80–100%*
End	Frontier technology	0.18	2040	2035	2030	0%	25–75%*
R	Near-term mature	0.3	2030	2028	2025	52%	80–90%*

*Note: The saturation penetration rate range corresponds to the values under the BAU to TBS scenarios; for the CUS scenario, the midpoint of the range ±25% is used.

(6) Scenario technology penetration rates

The technology penetration rates (%) for the base year 2023 and the year 2050 under each scenario are shown in Table S14.

Table S14 Technology penetration rates across scenarios

Technology ID	2023	BAU 2050	ESP 2050	TBS 2050	CUS 2050
S1	0	25	50	75	50–75
S2	0	25	50	75	50–75
E1	0	25	50	75	50–75
E2	0	25	50	75	50–75
T1	3	50	95	100	80–100
T2	35	100	100	100	80–100
T3	54	100	100	100	90–100
T4	26	95	100	100	90–100
T5	11	80	90	100	60–100
T6	8	60	90	100	50–100
T7	2	20	50	60	20–60
T8	26	80	90	100	70–100
End	0	25	50	75	50–75
R	52	80	90	90	80–90

2.5.2 MINLP Multi-objective Optimization Model (NSGA-II)

(1) Problem definition and decision variables

The penetration rates of the 14 emission reduction technologies are set as continuous decision variables X_j (j = 1, 2, ..., 14), with parameters assigned differentially across the eight coal chemical subsectors i. The optimization objective focuses on synergistically maximizing carbon emission reduction potential, pollutant reduction potential, and cost effectiveness.

Carbon emission reduction potential $$Max\ f_1 = \sum_{i=1}^{8} \sum_{j=1}^{14} CE_{ij} \times X_j \quad (22)$$

Pollutant reduction potential $$Max\ f_2 = \sum_{i=1}^{8} \sum_{j=1}^{14} PE_{ij} \times X_j \quad (23)$$

Cost effectiveness $$Max\ f_3 = \sum_{i=1}^{8} \sum_{j=1}^{14} \Delta C_{ij} \times X_j \quad (24)$$

Where, CE_{ij}, PE_{ij} and ΔC_{ij} represent the unit emission reduction potential, pollutant reduction potential, and net benefit of technology j applied in subsector i, respectively. The corresponding parameter matrices are provided in the industry technical parameter table.

(2) Constraints

The constraint system comprises 15 conditions across four categories: technology mutual exclusivity, capacity upper bounds, non-negativity, and staged emission reduction targets.

For technology mutual exclusivity:

Feedstock substitution technologies must satisfy: X1+X2≤100%

CCUS coupling and pure CCUS shall not be double-counted: X2+X13≤100%

The cumulative share of energy structure technologies cannot exceed 100%: X3+X4≤100%

Overlay constraint for electrification, direct green electricity supply, and intelligent load regulation: X3+X4+X6≤100%

Extended constraint for electrification, direct green electricity supply, intelligent load regulation, and waste heat recovery: X3+X4+X6+X10≤100%

For capacity constraints:

The output of each subsector shall not exceed 90% of the smaller value between traditional capacity and projected modern coal chemical capacity: $Q_i \leq 0.9 \times \min(CAP_{trad,i}, CAP_{modern,i}^{projected})$。

Non-negativity constraints require that all technology penetration rates remain non-negative, i.e., $X_j \geq 0$ for all j. Staged emission reduction targets stipulate that the carbon intensity in 2030 must decline by more than 65% relative to the 2005 level, which translates to $EI_{2030}/EI_{2005} \leq 0.35$.

(3) NSGA-II algorithm settings

We employed the NSGA-II algorithm to solve the mixed-integer nonlinear programming problem described above. The parameter settings were as follows. The population size was set to 200, and the maximum number of generations was 300. The algorithm was terminated early if the Pareto front showed no significant change over 50 consecutive generations. Crossover was performed using simulated binary crossover (SBX) with a probability of 0.9 and a distribution index η_c of 15. Polynomial mutation was applied with a probability of 0.05 and a distribution index η_m of 20. A binary tournament selection operator of size 2 was used. The elitism strategy preserved the best solutions by merging parent and offspring populations and retaining the superior individuals, thereby preventing population degradation.

(4) Convergence and parameter sensitivity analysis

Convergence was assessed using three metrics: generational distance (GD), hypervolume (HV), and spacing (SP). GD measures the proximity of the current front to the true front, with convergence deemed achieved when its rate of change falls below 0.1%. HV reflects the coverage range and quality of the front, while SP evaluates the uniformity of solution distribution. Under the settings of population size 200 and 300 generations, GD stabilized at generation 235, the HV increment was approximately 0.03% per generation, and SP remained below 0.05, indicating effective convergence of the algorithm. Parameter sensitivity tests were conducted under two configurations, one with population 150 and 200 generations, and the other with population 250 and 400 generations. The Hausdorff distances between the resulting Pareto fronts were all below 2%, confirming that the parameter settings lie within a reasonable range and that the optimization results are robust.