

Supporting Information

Sustainability analysis for the wastewater treatment technical route for coal-to-synthetic-natural-gas industry through zero liquid discharge vs. standard liquid discharge

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Table S1. Water quality of fix-bed coal gasification wastewater

Type	Pollutants	Concentration (mg/L)
Insoluble oils	Middle oils	12000
	Tar	15000
Sour gases	CO ₂	4500
	H ₂ S	300
Ammonia nitrogen	Ammonia	8000
Phenols	Phenol	2000
	Methylphenol	1000
	Dimethylphenol	200
	Trimethylphenol	150
	Ethylphenol	150
	O-dihydroxybenzene	600
	Resorcin	500
	Hydroquinone	1500
	Methyl diphenol	150
	Polyphenols	300
Heterocyclic compounds	Indoline	150
	Pyridine	100
	Quinoline	1100
	Imidazole	100
MAHs and PAHs	Benzene	300
	Methylbenzene	200
	Ethylbenzene	250
	Biphenyl	50
	Naphthalene	20
Long-chain alkanes		450
Fatty acids	Acetic acid	600
	Propionic acid	200
	Butyric acid	200
	Valeric acid	200
	Hexanoic acid	200

Table S2. Mass balance of wastewater treatment process

Number	Flow (t/h)	Insoluble oils(mg/L)	Acid gas(mg/L)	Ammonia Nitrogen(mg/L)	Total phenols(mg/L)	Heterocyclic compounds(mg/L)	Maps & Haps(mg/L)	Long chain alkanes(mg/L)	Fatty acids(mg/L)
1	1800	27000	4800	8000	6500	1450	820	450	1400
2	700	300	4800	8000	6500	1450	820	450	1400
3	1100	300	50	8000	450	1450	820	450	1400
4	1100	50	-	200	5	650	120	230	860
5	1100	-	-	50	1	80	10	40	-
6	1100	-	-	20	-	15	2	10	-
7	140	-	-	25	0.2	20	1.7	8.6	51
8	960	-	-	12	0.1	7	1	5	5
9	112	-	-	15	0.2	-	-	-	24
10	1072	-	-	12	-	7	1	5	6
11	28	-	-	-	-	-	-	-	-

Table S3. Reuse water quality indexes

Items	Control indexes	units
pH	6.5-8.5	-
COD	40	mg/L
Ammonia nitrogen	5	mg/L
Total phenols	0.2	mg/L
Heterocyclic	5	mg/L
Long-chain alkanes	5	mg/L
Fatty acids	5	mg/L
TDS	400	mg/L
Turbidity	3	NTU
Suspended solids	10	mg/L
Total hardness	300	mg/L
Total alkalinity	250	mg/L
Chloridion	100	mg/L
Total phosphorus	1	mg/L

Table S4. Summary of detailed inventory for SLD and ZLD

	Unit	T1	T2	T3	T4	T5	T6
Inputs							
Wastewater 1	t	1800	1052	1030	1026.5	1026	136
Electricity	kWh	3626	1650	5689	550	270	3000
MIBK	kg	-	300	-	-	-	-
PAM	kg	-	-	10.894	4.921	-	-
Defoaming agent	kg	-	-	25.419	-	-	-
NaClO	kg	-	-	-	31.845	-	8.75
PAC	kg	-	-	6.875	330.507	8.25	-
Activated coke	kg	-	-	-	1.747	-	-
Scale inhibitors	kg	-	-	-	-	9.375	9.375
Reducing agent	kg	-	-	-	-	17.5	2.5
Fungicide	kg	-	-	-	-	4.375	-
HCl	kg	-	-	-	-	-	8.75
NaOH	kg	-	1800	-	-	-	62.5
Steam	t	42(0.5)	46(0.5),136(1.5),20(4.7)		-	-	40(0.5)
CaSO ₄	kg	-	-	-	-	-	375
Outputs							
Wastewater 2	t	700	-	-	-	-	-
Treated wastewater	t	1052	1030	1026.5	1026	136	-
Insoluble oils	t	48	-	0.515	-	-	-
Acid gas	t	-	5	0.515	-	-	-
Ammonia nitrogen	kg	-	8210	154.5	30.8	-	-
Total phenols	kg	-	6410	458.35	4.11	-	-
Heterocyclic compounds	kg	-	840	1617.1	66.7	-	-

MAPs and HAPs	kg	-	740	113.3	8.21	-	-
Long chain alkanes	kg	-	230	195.7	30.8	-	-
Fatty acids	kg	-	570	885.8	-	-	-
Wet coke	t	-	-	-	4.24	-	-
Sludge	m ³	-	-	5.54	-	-	-
Salts	t	-	-	-	-	-	27.2
Reused water	t	-	-	-	-	890	108.8

Table S5. Estimation coefficients of the total production cost

Component	Reference value	Design value
(1) Operating costs		
(1.1) Direct costs		
(1.1.1) Raw material	10~50% of production cost	Calculated value
(1.1.2) Operating labor	10~20% of production cost	300 labors 30000CNY/labor/year
(1.1.3) Regulatory costs	10~20% of operating labor	15% of operating labor
(1.1.4) Utilities	10~20% of production cost	Calculated value
(1.1.5) Maintenance and repairs	2~10% of capital investment	10% of capital investment
(1.1.6) Operating supplies	0.5~1% of capital investment	0.75% of capital investment
(1.1.7) Laboratory charge	10~15% of operating labor	10% of operating labor
(1.2) Fixed expenses		
(1.2.1) Depreciation	As appropriate	Life period 20 years, salvage value 4%
(1.2.2) Tax	1~4% of capital investment	4% of capital investment
(1.2.3) Insurance	0.4~1% of capital investment	0.7% of capital investment
(1.2.4) Rent	8~12% of buildings and land	10% of buildings and land
(1.3) Plant overhead costs	5~15% of direct costs	10% of direct costs
(2) Daily costs		
(2.1) Administrative costs	2~6% of production cost	4% of production cost
(2.2) Distribution and selling costs	2~20% of production cost	4% of production cost
(2.3) Research cost	2~5% of production cost	2% of production cost
(2.4) Financial cost	0~10% of total capital investment	2% of total capital investment
(3) Production cost	(1)+(2)	(1)+(2)

Table S6. Percentage of investment components

Component	Value range (%)	Calculated value (%)
(1) Direct investment		
(1.1) Equipment	15~40	21
(1.2) Installation	6~14	10
(1.3) Instruments and controls	2~8	5
(1.4) Piping	2~20	12
(1.5) Electrical	2~10	6
(1.6) Buildings (including services)	3~18	15
(1.7) Land	1~2	1
(2) Indirect investment		
(2.1) Engineering and supervision	4~21	10
(2.2) Construction expenses	3~16	9
(2.3) Contractor's fee	2~6	4
(2.4) Contingency	5~15	7
(3) Fixed capital investment	(1)+(2)	100
(4) Working capital	10~20	17
(5) Total capital investment	(3)+(4)	117

Table S7. Unit external cost of pollutant emissions

Pollutants	Unit external cost (CNY/kg)
CO ₂	0.195
CH ₄	1.46
PM _{2.5}	156
NO _x	31.9
SO ₂	24.5
CO	4.15

Table S8. Equivalent factor of GHG emissions (100 years)

GHG	CF (kg CO ₂ -eq/kg)
CO ₂	1
N ₂ O	298
CH ₄	25

Table S9. Weighting factor by environment and human health impact categories

Categories	Environment impact					Human health impact	
	GWP	AP	EP	ADP	POCP	HCP	HNCP
Weighting factor	0.644	0.124	0.149	0.044	0.039	0.750	0.250