
Supplementary Materials

Highly efficient CO₂ capture and utilization of coal and coke-oven gas
coupling for urea synthesis process integrated with chemical looping
technology: Modeling, parameters optimization, and performance analysis

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The calculation of the total capital investment is based on the calculation of the ratio factor of the FCI and the component capital investment, expressed as follows:

Table S1. Ratio factors for capital investment.

Component	Range (%)	Assumed value (%)
(1) Direct investment		
(1.1) Equipment	16–40	30
(1.2) Equipment installation	7–14	8
(1.3) Piping	3–9	5
(1.4) Electrical systems	2–10	6
(1.5) Buildings (including services)	5–16	12
(1.6) Instruments and controls	2–7	5
(1.7) Land	1–2	1
(2) Indirect investment		
(2.1) Engineering and supervision	4–19	11
(2.2) Construction expenses	4–18	10
(2.3) Contractor's fee	2–7	5
(2.4) Contingency	5–17	7
(3) Fixed capital investment	(1) + (2)	100
(4) Working capital	10–20	15
(5) Total capital investment	(3) + (4)	115

The total production cost includes the raw material costs, utility consumption, labor costs, factory depreciation and residual value, administrative investment, and maintenance and operating costs. The main assumptions are shown as follows:

Table S2. Assumptions for the estimation of the total product cost.

Component	Basis
(1) Raw material	coal: 100 US\$/t, COG: 0.06 US\$/m ³
(2) Utilities	water: 0.3 US\$/t, electricity: 0.7 US\$/kWh, steam: 6.0 US\$/GJ, natural gas: 0.3 US\$/Nm ³
(3) Operating & Maintenance	
(3.1) Operating labor	300 labors, 100000 CNY/labor/year
(3.2) Supervisory and clerical labor	20% of operating labor
(3.3) Maintenance and repairs	2% of fixed capital investment

(3.4) Operating supplies	0.7% of fixed capital investment
(3.5) Laboratory charge	15% of operating labor
(4) Depreciation	Life period 15 y, salvage value 4%
(5) Plant overhead cost	60% (3.1+3.2+3.3)
(6) Administrative cost	2% of product cost
(7) Distribution and selling cost	2% of product cost
(8) Product cost	(1)+(2)+(3)+(4)+(5)+(6)+(7)

Main simulation data of CTU, CTU_{CLAS&H}, and COG-CTU_{CLAS&H} processes

are shown as follows:

Table S3. Simulation results of the CTU process.

Stream No.	1	2	3	4	5	6	7
Molar fraction (%)							
CO	-	43.82	1.05	-	-	-	-
CO ₂	-	8.08	40.14	-	-	32.97	-
H ₂	-	30.41	58.12	75.13	0.82	-	-
H ₂ O	-	17.14	0.26	-	-	-	0.99
N ₂	-	0.26	0.21	24.87	0.18	-	-
H ₂ S+SO _x	-	0.29	0.19	-	-	-	-
NH ₃	-	-	-	-	99.00	66.03	-
Urea	-	-	-	-	-	-	99.01
Molar flow (kmol/h)	-	19591.76	24571.38	19366.10	9231.04	13904.15	3766.42
Coal (tonne/h)	200	-	-	-	-	-	-
Temperature (°C)	40	1350	40	38	200	100	72
Pressure (MPa)	0.1	6.5	0.1	1.2	6.5	14	14

Table S4. Simulation results of the CTU_{CLAS&H} process.

Stream No.	1	2	3	4	5	6	7
Molar fraction (%)							
CO	-	41.28	~0	-	-	-	-
CO ₂	-	10.13	64.56	-	-	31.34	-
H ₂	-	27.45	~0	74.97	1.17	0.81	-
H ₂ O	-	20.61	35.37	0.16	0.33	0.22	0.98
N ₂	-	0.26	0.07	24.88	0.29	0.20	-
H ₂ S+SO _x	-	0.24	-	-	-	-	-
NH ₃	-	-	-	-	98.21	67.43	-
Urea	-	-	-	-	-	-	99.02
Molar flow (kmol/h)	-	11869.4	9370.38	9367.22	8042.37	6892.15	2185.86
Coal (tonne/h)	120	-					

Temperature (°C)	40	1350	40	40	200	100	72
Pressure (MPa)	0.1	6.5	0.1	3.0	6.5	14	14

Table S5. Simulation results of the COG-CTU_{CLAS&H} process.

Stream No.	1	2	3	4	5	6	7
Molar fraction (%)							
CO	-	6.70	41.28	~0.00	-		-
CO ₂	-	2.00	10.13	52.34	-	33.14	-
H ₂	-	58.00	27.45	~0.00	74.79	0.43	-
H ₂ O	-	-	20.61	47.76	~0.00	0.24	0.54
N ₂	-	0.30	0.26	~0.00	25.21	0.41	-
O ₂		4.00					
CH ₄		27.00					
H ₂ S+SO _x	-	2.00	0.24	-	-	-	-
NH ₃	-	-	-	-	-	65.78	-
Urea							99.46
Molar flow (kmol/h)	-	22258.12	11869.4	19451.71	8042.37	14191.21	8026.85
Coal (tonne/h)	120						
Temperature (°C)	40	1354	1350	40	200	100	72
Pressure (MPa)	0.1	6.5	6.5	0.1	6.5	14	14