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Ethylene production from shale gas using a dielectric barrier discharge plasma reactor: an integrative circular economy perspective

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Supplementary Material

A. Experimental basis for kinetic model development

Table S1. Experimental outlet compositions used for lumped kinetic model development.

Run	Voltage [kV]	Frequency [kHz]	Discharge Power [W]	CH_4 Inflow [sccm]	H_2	CH_4	C_2H_6	C_2H_4	C_2H_2	C_3H_8	C_3H_6	C_4H_{10}	C_5H_{12}	C
0	15	1	37	30	9.804	84.304	2.551	0.174	0.142	0.768	0.043	0.124	0.131	1.96
1	15	1	37	50	6.437	89.628	1.836	0.149	0.119	0.525	0.031	0.078	0.087	1.108
2	15	1	37	70	4.774	92.291	1.399	0.133	0.101	0.382	0.025	0.053	0.062	0.781
3	15	1	37	90	3.774	93.898	1.122	0.121	0.088	0.295	0.02	0.039	0.047	0.597

Table S2. Lumped reaction network and kinetic constants obtained for the DBD methane conversion model.

				$(mol/s/bar^n/m^3)$
0	2CH4 -> C2H6 + H2	r0 = k0*P_CH4^2	k0	9.51E-02
1	C2H6 -> C2H4 + H2	r1 = k1*P_C2H6	k1	3.85E-01
2	C2H4 + H2 -> C2H6	r2 = k2*P_C2H4*P_H2	k2	1.96E-07
3	2CH4 -> C2H4 + 2H2	r3 = k3*P_CH4^2	k3	4.22E-02
4	C2H4 + 2H2 -> 2CH4	r4 = k4*P_C2H4*P_H2^2	k4	1.71E-03
5	C2H4 -> C2H2 + H2	r5 = k5*P_C2H4	k5	2.97E+00
6	C2H4 + CH4 -> C3H8	r6 = k6*P_CH4*P_C2H4	k6	2.48E+01
7	C3H8 -> C3H6 + H2	r7 = k7*P_C3H8	k7	2.74E-01
8	C3H6 -> C2H2 + CH4	r8 = k8*P_C3H6	k8	2.49E-10
9	2C2H4 + H2 -> C4H10	r9 = k9*P_C2H4^2*P_H2	k9	2.04E-02
10	C3H8 + CH4 -> C4H10 + H2	r10 = k10*P_C3H8*P_CH4	k10	2.10E+00
11	C4H10 + CH4 -> C5H12 + H2	r11 = k11*P_C4H10*P_CH4	k11	7.49E+00

Table S3. Electron-impact reaction set considered in the kinetic derivation.

	Reaction	Category
0	e+CH4 -> e+CH4	Elastic/momentum transfer
1	e+CH3 -> e+CH3	
2	e+CH2 -> e+CH2	
3	e+C2H6 -> e+C2H6	
4	e+C2H4 -> e+C2H4	
5	e+C2H2 -> e+C2H2	
6	e+C3H8 -> e+C3H8	
7	e+C3H6 -> e+C3H6	
8	e+CH4<->e+CH4(v13)	Vibrational excitation
9	e+CH4<->e+CH4(v12)	
10	e+C2H6<->e+C2H6(v24)	
11	e+C2H6<->e+C2H6(v13)	
12	e+C2H4<->e+C2H4(v1)	
13	e+C2H4<->e+C2H4(v2)	
14	e+C2H2<->e+C2H2(v13)	
15	e+C2H2<->e+C2H2(v2)	

16	e+C2H2<->e+C2H2(v5)	
17	e+C3H8<->e+C3H8(v1)	
18	e+C3H8<->e+C3H8(v2)	
19	e+C3H6<->e+C3H6(v)	
20	e+CH4->e+CH3+H	Electron-impact dissociation
21	e+CH4->e+CH2+H2	
22	e+CH4->e+C+2H2	
23	e+C2H6->e+C2H4+H2	
24	e+C2H4->e+C2H2+H2	
25	e+C2H4->e+C2H3+H	
26	e+C3H8->e+C3H6+H2	
27	e+C3H6->e+C2H2+CH4	
28	e+CH4<->2e+CH4+	Electron-impact ionization
29	e+CH3<->2e+CH3+	
30	e+C2H6<->2e+C2H6+	
31	e+C2H4<->2e+C2H4+	
32	e+C2H2<->2e+C2H2+	
33	e+C3H8<->2e+C3H8+	
34	e+C3H6<->2e+C3H6+	
35	e+C2H5+=>C2H2+H+H2	
36	e+C2H5+=>C2H3+2H	
37	e+C2H5+=>C2H2+3H	

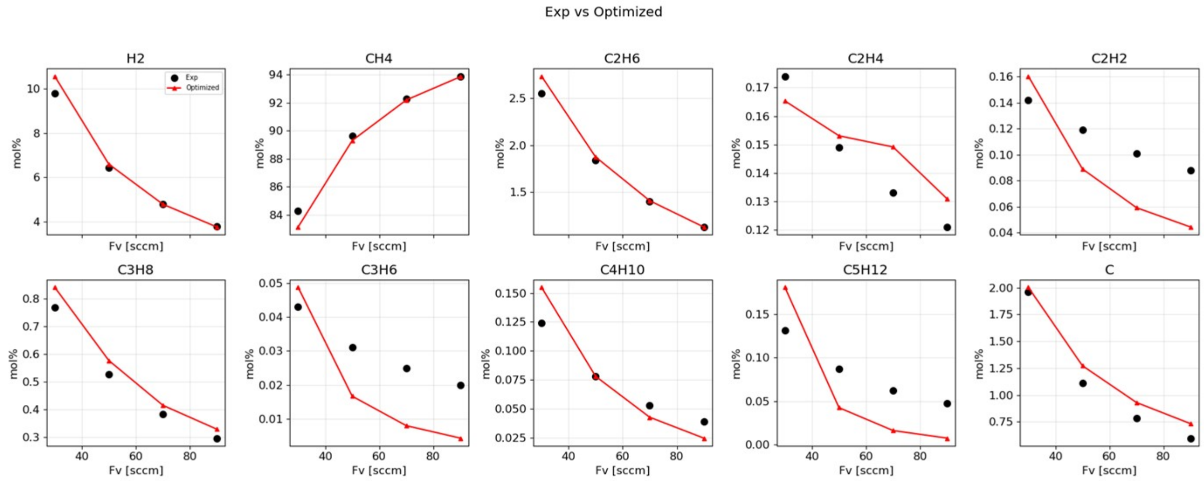

Fig S1. Comparison of experimental and predicted outlet compositions at different CH_4 inflow rates.

B. Feed gas composition

Table S4. Shale gas composition assumed in the present design.

Components	Composition (% by volume)
CH_4	92.61
C_2H_6	3.78
C_3H_8	1.42
C_4H_{10}	0.04
iso-C_4H_{10}	0.02
C_5H_{12}	0.02
iso-C_5H_{12}	0.01
C_6H_{14}	0.01
N_2	1.35
CO_2	0.67
CO	0.03
O_2	0.03
H_2S	0.01

C. Heat integration result

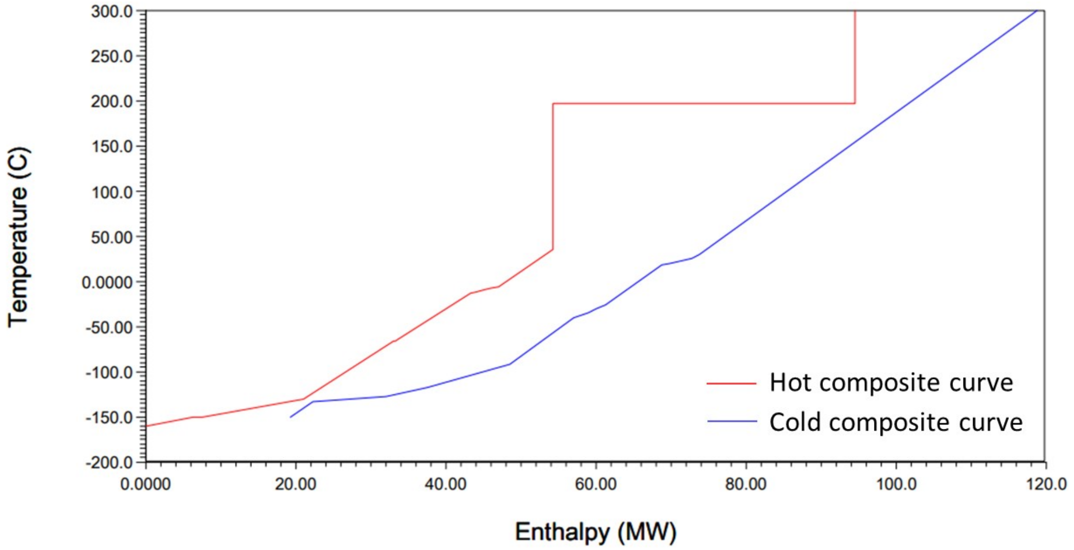

Fig S2. Composite curves for base case(On-site feed gas).

D. Process stream and equipment information

Table S5. Process major stream information.

Component	Unit	12	RXN	16	17	18	21	24	28	13-2	30	31
H_2	kmol/hr	-	-	4914.8	4914.8	45.5	69.3	-	118.9	57.9	0.1	57.9
N_2	kmol/hr	5856	5856	5856	5856	-	5856	2.6	3.4	3.4	0.2	3.4
CO_2	kmol/hr	-	-	3.3	-	-	-	3.3	3.3	3.3	-	3.3
CO	kmol/hr	2.3	2.3	37.8	37.8	-	-	37.8	37.8	37.8	-	37.8
C (Cokes)	kmol/hr	-	-	1630.7	-	-	-	-	-	-	-	-
CH_4	kmol/hr	5497.6	4247.6	3316.8	3316.8	-	-	136.8	6.8	3336.8	0.1	1.8
C_2H_2	kmol/hr	-	-	173.2	173.2	-	-	173.2	173.2	-	-	-
C_2H_4	kmol/hr	-	-	175	175	-	-	175	175	346.5	141.4	205.1
C_2H_6	kmol/hr	224.9	224.9	63.6	63.6	-	-	63.6	63.6	65.3	1.2	65.3
C_3H_8	kmol/hr	84.3	84.3	13.6	13.6	-	-	13.6	13.6	1.5	-	13.6
C_4H_{10}	kmol/hr	2.3	2.3	1.8	1.8	-	-	1.8	1.8	0.5	-	1.8
C_5+	kmol/hr	1.2	1.2	2.5	2.5	-	-	2.5	2.5	1.2	-	2.5
Olefins	kmol/hr	1.2	1.2	24.9	24.9	-	-	24.9	24.9	24.9	-	24.9

E. Economic analysis

Table S6. List of major economic parameters and assumptions.

Shale gas prices ($ per ton)	32.45
Methane (off-site pipeline gas) price ($ per ton) [a]	200.0
Nitrogen (off-site pipeline gas) price ($ per ton) [a]	150.8
Pd/WS_2 catalyst price ($ per ton) [c]	58.8
aMDEA price ($ per ton) [c]	3006.8
Triethylene glycol price ($ per ton) [c]	1200.9
Alumina price ($ per ton) [c]	400.5
Waste disposal ($ per ton) [b]	38.5
Wastewater treatment chemical price ($ per ton) [e]	5778.4
Electricity price ($ per kWh) [e]	0.07
Steam price ($ per kWh) [f]	0.04
Discount rate (%)	10.0
Plant financing by equity (%) [e]	40.0
Plant life (years) [e]	30.0
Income tax rate (%) [e]	35.0
Interest rate for debt financing (%) [e]	8.0
Term for debt financing (years) [e]	10.0
General plant depreciation (years) [e]	7.0
Working capital (% of fixed capital investment) [e]	5.0
On-stream percentage after startup (%) [e]	90.0
Startup time (years) [e]	0.25
Revenue and costs during startup	
Revenue (% of normal) [e]	50.0
Variable costs (% of normal) [e]	75.0
Fixed costs (% of normal) [e]	100.0
Construction period (years) [e]	3.0
First 12 months' expenditures (%) [e]	8.0
Next 12 months' expenditures (%) [e]	60.0
Last 12 months' expenditures (%) [e]	32.0

[a] Taken from Humbird et al. (2011)
[b] Taken from Davis et al. (2018)
[c] Taken from Liu et al. (2015)
[d] Taken from Kazi et al. (2010)
[e] Taken from Davis et al. (2015)
[f] Taken from Motagamwala et al. (2018)

F. First-of-a-Kind (FOAK) plant analysis

Table S7. Parameters and equations used in pioneer plant analysis.

Parameter	Definition	Range	Value
Plant performance [a]		0–89	25
	$= g(process\ maturity, ope$ $\times BALEQS - 4.12 \times WASTE$		
NEWSTEPS	Number of new process steps based on block	≥ 0	3
BALEQS [a]	Percentage of heat and mass balance equations based on actual prior plant data	0–100	20
WASTE [b]	Factor for waste handling encountered during development	0–5	2
SOLIDS [b]	Factor for presence of solid feedstock or products	0 or 1	1
Cost growth		>0	0.52
	$= f(technology\ complexit$ $- 0.02125 \times IMPURITIES$ $- 0.06361 \times PROJECT\ DEF$		
PCTNEW	Estimate (%) of unproven technology incorporated in commercial use	0–100	40
IMPURITIES [c]	Factor for impurities present in process	0–5	2
COMPLEXITY [d]	Block count of all process steps in plant	≥ 1	6
INCLUSIVENESS [c]	Percentage of three factors: pre-startup personnel costs, pre-startup inventory cost, and land purchase	0–100	100
PROJECT DEFINITION [d]	Levels of site-specific information and engineering included in estimate	2–8	7
[a]	Taken from Rubin et al. (2021)		
[b]	Taken from Baccarini (2006)		
[c]	Taken from Jia et al. (2010)		
[d]	Taken from Loose et al. (2024)		

G. Project cost

Table S8. Result of project cost calculation.

Areas			Installed cost ($)
Acid gas removal			35,393,754
TEG dehydration			2,108,810
Plasma reaction			14,337,491
PSA			16,873,696
LPG separation			4,556,420
Ethylene production			2,347,876
ISBL (inside battery limits)			**75,618,046**
Wastewater treatment			1,968,330
Storage			2,906,965
Heat and power generation			134,630,108
Utilities			38,060,602
OSBL (outside battery limits)			**177,566,005**
Total installed equipment			**253,184,051**
Warehouse	4%	of ISBL	3,024,722
Site development	9%	of ISBL	6,805,624
Additional piping	5%	of ISBL	3,780,902
TDC (total direct costs)			**266,795,299**
Prorateable expenses	10%	of TDC	26,679,530
Field expenses	10%	of TDC	26,679,530
Home office & construction fee	20%	of TDC	53,359,060
Project contingency	10%	of TDC	26,679,530
Other costs (start-up, permits, etc)	10%	of TDC	26,679,530
TIC (total indirect costs)			**160,077,179**
FCI (fixed capital investment)			**456,660,152**
Land	2%	of FCI	9,133,203
Working capital	5%	of FCI	22,833,008
TCI (total capital investment)			**488,626,362**

Table S9. Detailed equipment cost basis for major process units.

Section	Equipment / service	Design basis or sizing basis	Base capacity or flow (kg/h)	Actual capacity or flow (kg/h)	Scaling exponent	Purchased cost, base year ($)	Base year	Purchased cost, project year ($)	Installation factor	Installed cost, project year ($)
Acid gas removal	AGRU	Feed gas throughput	223,000	407,349	0.6	13,127,000	2018	22,121,096	1.6	35,393,754
TEG dehydration	TEG unit	Dehydration gas throughput	1,055.7	276,385.8	0.7	21,400	2021	1,054,405	2.0	2,108,810
LPG separation	Demethanizer	Hydrocarbon separation train	416,544	41,440	0.6	1,450,000	2020	453,764	1.6	726,023
	Deethanizer	Hydrocarbon separation train	416,544	41,440	0.6	1,200,000	2020	375,529	1.6	600,847
	Debutanizer	Hydrocarbon separation train	416,544	41,440	0.6	1,000,000	2020	312,941	1.6	500,705
	Cryogenic compressor	Hydrocarbon separation train	416,544	41,440	0.6	2,750,000	2020	860,588	1.6	1,376,940
	Heat exchanger	Hydrocarbon separation train	416,544	41,440	0.6	800,000	2020	250,353	1.6	400,564
	Refrigeration system	Hydrocarbon separation train	416,544	41,440	0.6	1,900,000	2020	594,588	1.6	951,341
Ethylene production	Fixed-bed reactor	Hydrogenation section throughput	5,600	504.2	0.6	1,200,000	2025	283,032	2.2	622,669
	Pd-Ag/α-Al2O3 catalyst system	Hydrogenation section throughput	5,600	504.2	0.6	400,000	2025	94,344	1.5	141,516
	Feed preheater	Hydrogenation section throughput	5,600	504.2	0.6	150,000	2025	35,379	2.2	77,834
	Intercooler	Hydrogenation section throughput	5,600	504.2	0.6	120,000	2025	28,303	2.2	62,267
	Hydrogen compressor	Hydrogenation section throughput	5,600	504.2	0.6	300,000	2025	70,758	2.3	162,743
	Gas chromatograph	Hydrogenation section throughput	5,600	504.2	0.6	250,000	2025	58,965	1.8	106,137
	Control system (APC)	Hydrogenation section throughput	5,600	504.2	0.6	500,000	2025	117,930	1.5	176,895
	Pressure relief system	Hydrogenation section throughput	5,600	504.2	0.6	100,000	2025	23,586	2.0	47,172
	C2H4-PSA	Hydrogenation section throughput	5,600	504.2	1.0	1,200,000	2025	108,045	2.2	237,699
	Packaged auxiliaries and controls	Integrated ethylene finishing package	–	–	–	–	2021	396,080	1.8	712,944
Wastewater	Neutralization +	Wastewater flow	100,000	13,220	0.6	800,000	2011	302,820	1.6	484,512

treatment	settler									
	Organic removal (UF)	Wastewater flow	100,000	13,220	0.6	950,000	2011	359,599	1.6	575,358
	RO + polishing unit	Wastewater flow	100,000	13,220	0.6	1,500,000	2011	567,788	1.6	908,460
Storage	LPG storage tank	Product storage throughput	416,544	41,440	0.6	1,200,000	2020	375,529	2.0	751,058

H. Discounted cash flow analysis

Table S10. Discounted cash flow calculations.

Year	-2	-1	0	1	2	3	4	5	6	7	8
Fixed capital investment	14,613,125	109,598,436	58,452,499								
Land	9,133,203										
Working capital			22,833,008								
Loan payment				40,833,497	40,833,497	40,833,497	40,833,497	40,833,497	40,833,497	40,833,497	40,833,497
Loan interest payment	1,753,575	14,905,387	21,919,687	21,919,687	20,406,582	18,772,429	17,007,544	15,101,468	13,042,905	10,819,658	8,418,551
Loan principal	21,919,687	186,317,342	273,996,091	255,082,281	234,655,366	212,594,298	188,768,345	163,036,315	135,245,723	105,231,883	72,816,936
C_2H_4 sales				409,777,493	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991
LPG sales				294,988,500	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000
C_5+ condensate sales				84,645,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000
Total annual sales				397,045,171	789,410,993	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991
Annual manufacturing cost											
Feedstock				288,685,332	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776
Electricity				350,031,476	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900
Solvent				66,858,334	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445
Catalyst				4,422,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000
Diluent				20,787,536	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715
Other variable operating costs				42,965,006	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864
Fixed operating costs				4,395,540	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475
Total product cost				778,145,223	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174
Annual depreciation											
General plant writedown				14%	24%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%
Depreciation charge				65,256,736	111,836,071	79,869,861	57,036,853	40,779,752	40,734,086	40,779,752	20,367,043
Remaining value				391,403,416	279,567,345	199,697,484	142,660,631	101,880,880	61,146,794	20,367,043	0
Net revenue				-75,910,653	-61,690,836	-28,090,473	-3,492,580	14,670,598	16,774,826	18,952,408	41,766,224
Losses forward					-75,910,653	-137,601,489	-165,691,962	-169,184,542	-154,513,944	-137,739,117	-118,786,709
Taxable income				-75,910,653	-137,601,489	-165,691,962	-169,184,542	-154,513,944	-137,739,117	-118,786,709	-77,020,486
Income tax				0	0	0	0	0	0	0	0
Annual cash income				-29,567,727	29,718,320	29,718,320	29,718,320	29,718,320	29,718,320	29,718,320	29,718,320
Discount factor	1.210	1.100	1.000	0.826	0.683	0.5645	0.4665	0.3855	0.3186	0.2633	0.2176
Annual present value				-24,436,138	20,298,012	16,775,217	13,863,816	11,457,699	9,469,173	7,825,762	6,467,572
Total capital investment + interest	37,334,408	150,649,627	103,205,194								
Net present worth			0								

Year	9	10	11	12	13	14	15	16	17	18	19
Fixed capital investment											
Land											
Working capital											
Loan payment	40,833,497	40,833,497	0	0	0	0	0	0	0	0	0
Loan interest payment	5,825,355	3,024,704	0	0	0	0	0	0	0	0	0
Loan principal	37,808,794	0	0	0	0	0	0	0	0	0	0
C_2H_4 sales	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991
LPG sales	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000
C_5+ condensate sales	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000
Total annual sales	529,393,562	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991
Annual manufacturing cost											
Feedstock	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776
Electricity	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900
Solvent	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445
Catalyst	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000
Diluent	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715
Other variable operating cost	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864
Fixed operating costs	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475
Total product cost	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174
Annual depreciation											
General plant writedown											
Depreciation charge											
Remaining value											
Net revenue	64,726,462	67,527,114	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817
Losses forward	-77,020,486	-12,294,023	0	0	0	0	0	0	0	0	0
Taxable income	-12,294,023	55,233,090	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817
Income tax	0	16,569,927	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545
Annual cash income	29,718,320	13,148,393	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272
Discount factor	0.1799	0.1486	0.1228	0.1015	0.0839	0.0693	0.0573	0.0474	0.0391	0.0323	0.0267
Annual present value	5,345,101	1,954,425	6,066,905	5,013,971	4,143,778	3,424,610	2,830,256	2,339,054	1,933,103	1,597,606	1,320,335
Total capital investment + interest											
Net present worth											

Year	20	21	22	23	24	25	26	27	28	29	30
Fixed capital investment											
Land											
Working capital											
Loan payment	0	0	0	0	0	0	0	0	0	0	0
Loan interest payment	0	0	0	0	0	0	0	0	0	0	0
Loan principal	0	0	0	0	0	0	0	0	0	0	0
C_2H_4 sales	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991	546,369,991
LPG sales	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000	393,318,000
C_5+ condensate sales	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000	112,860,000
Total annual sales	529,393,562	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991	1,052,547,991
Annual manufacturing cost											
Feedstock	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776	384,913,776
Electricity	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900	420,198,900
Solvent	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445	89,144,445
Catalyst	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000	5,896,000
Diluent	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715	27,716,715
Other variable operating cost	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864	49,102,864
Fixed operating costs	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475	5,023,475
Total product cost	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174	981,996,174
Annual depreciation											
General plant writedown											
Depreciation charge											
Remaining value											
Net revenue	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817
Losses forward	0	0	0	0	0	0	0	0	0	0	0
Taxable income	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817	70,551,817
Income tax	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545	21,165,545
Annual cash income	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272	49,386,272
Discount factor	0.0221	0.0183	0.0151	0.0125	0.0103	0.0085	0.0070	0.0058	0.0048	0.0040	0.0033
Annual present value	1,091,186	901,807	745,295	615,946	509,046	420,699	347,686	287,343	237,474	196,259	162,198
Total capital investment + interest											
Net present worth											

I. Life-cycle assessment

Table S11. LCA data of shale gas-to-ethylene process

Input	Amount	Unit	Database
Methane, high pressure (pipeline grade) {GLO}, 2022/kg/RNA	3.002	kg	ecoinvent 3.6
Nitrogen, liquid {GLO}| market for | Cut-off, U	2.099	kg	ecoinvent 3.6
Pd/WS_2 catalyst (1 wt% Pd)| market group for | Cut-off, U	0.102	kg	ecoinvent 3.6
Triethylene glycol (TEG), virgin {GLO}| market for | Cut-off, U	0.015	kg	ecoinvent 3.6
aMDEA (45 wt% aqueous solution), {GLO}| Cut-off, U	0.008	kg	ecoinvent 3.6
Alumina, activated {GLO}|/kg/RNA	0.019	kg	ecoinvent 3.6
Enzyme, Cellulase, Novozyme Celluclast/kg/RER	0.223	kg	ecoinvent 3.6
Heat, district or industrial, natural gas {GLO}| market group for | Cut-off, U	29.957	MJ	ecoinvent 3.6
Electricity, medium voltage {GLO}| market group for | Cut-off, U	5.405	MJ	ecoinvent 3.6
Output			
Ethylene, polymer grade	1.000	kg	ecoinvent 3.6
Carbon dioxide, biogenic	0.337	kg	ecoinvent 3.6
Carbon black	0.076	kg	ecoinvent 3.6
Vent gas (light ends)	1.041	kg	ecoinvent 3.6
Water	3.404	kg	ecoinvent 3.6
Dummy_Disposal, solid waste, unspecified, to unspecified landfill/kg/RNA	1.848	kg	USLCI

J. Sensitivity of pretreatment burden to shale gas composition variability

Table S12. Impact of shale gas compositions on the process economics.

	Raw shale gas CH_4 (mol%)	Relative AGR + TEG cost	Estimated MSP change (%)	Estimated MSP (\$/ton C_2H_4)
Low-CH_4 case	87.61	1.08	1.44	916.41
Base case	92.61	1.00	0.00	903.40
High-CH_4 case	97.61	0.96	-0.72	896.90

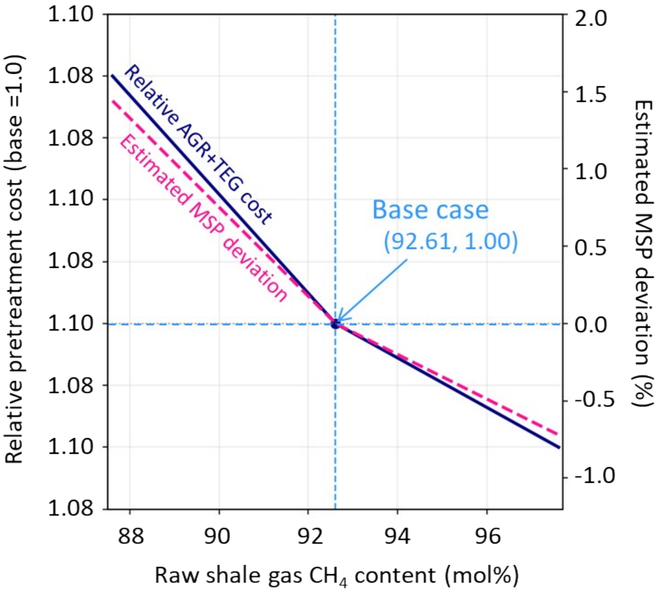

Fig S3. Sensitivity of pretreatment cost and propagated MSP to raw shale gas methane content.

To provide a quantitative indication of the potential economic effect of shale gas composition variability, a simple literature-informed sensitivity analysis was performed for the upstream pretreatment section. In the base design, the raw shale gas contains 92.61 mol% CH_4 and is conditioned through acid gas removal (AGR) and TEG dehydration prior to entering the plasma reactor. Because the reactor feed is defined after purification, variations in the raw shale gas composition are expected to affect primarily the pretreatment burden rather than the plasma reaction model or the downstream separation section itself. Previous shale gas processing studies have shown that raw gas composition variability can alter the burden of upstream treatment systems depending on methane content and impurity levels (He and You, 2014). In addition, dehydration studies have reported that higher acid gas content increases the water content of the treated gas and solvent losses, thereby increasing the burden of the TEG dehydration section (Perić et al., 2019), whereas the overall sensitivity of TEG systems is reflected mainly in operating burden rather than major changes in capital cost (Petropoulou et al., 2019).

Based on these observations, the methane content of the raw shale gas was varied by ± 5 mol% around the base composition, and the relative AGR + TEG pretreatment cost was conservatively varied from 0.96 to 1.08. The resulting propagated effect on the minimum selling price (MSP) was estimated using the pretreatment cost share in the overall process cost breakdown. As shown in Fig. S3, the relative pretreatment cost increases as the methane content of the raw shale gas decreases, while the corresponding MSP deviation remains limited. Across the examined range, the estimated MSP varies from −0.72% to +1.44% relative to the base-case MSP of $903.4/ton C_2H_4. These results suggest that shale gas composition variability can influence the upstream conditioning burden, but its contribution to the overall process economics remains secondary relative to the dominant cost drivers considered in the main uncertainty analysis.

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