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Deciphering the true life cycle environmental impacts and costs of the mega-scale shale gas-to-olefins projects in the United States

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1 Supply and production models

1.1 Shale regions and wells

Table S-1 Main shale regions in the United States [1, 2]

Region	Basin area (sq.miles)		Well spacing (wells/sq. mile)	EUR[a] (Bcf/well)	Well number	Ave. gas EUR (Bcf/well)	Ave. oil EUR[b] (MBO/well)	Ave. well spacing (sq. mile/well)
	Leased	Unleased						
Gulf Coast (GC)								
Eagle Ford	1090	-	4	5.00	4360			
Haynesville	3574	5426	8	3.57	72000	3.49	16.10	0.15
Floyd-Neal/Conasauga	2429	-	2	0.90	4858			
Subtotal	7093	5426			81218			
Mid-continent (MC)								
Woodford	4700	-	4	2.07	18800			
Woodford-Cana	688	-	4	5.20	2752	2.16	62.05	0.15
Fayetteville	9000	-	8	2.07	72000			
Subtotal	14388	-			93552			
Rocky Mountain (RM)								
Mancos	6589	-	8	1.00	52712			
Williston-Shallow [c]	NA	-	2	-	-	1.06	43.88	0.17
Lewis	7506	-	3	1.30	22518			
Bakken Shale Oil Play [d]	6522	-	1	0.75	6522			

Subtotal	20617				81752			
Appalachia (AP)								
Marcellus [e]	3541	28090	8	1.18	253048	0.97	0.35	0.13
Big Sandy	8675	1994	8	0.33	85352			
Subtotal	12216	30084			338400			

[a] To estimate a EUR of a well, the lifetime and initial production must be provided. However, this number is not clearly provided in the EIA report.[1] From some production decline curves present in this report, the average life time is assumed to 20 years.

[b] In the GC and RM shale regions, only Eagle Ford and Bakken shale plays have oil productions (300 and 500 MBO).[1] In addition, the oil EURs in the MC and AP shale regions are estimated based on the oil/gas ratio of 28.7 bbl/MMscf and 0.36 bbl/MMscf.[3]

[c] The Bakken shale oil play is located within the Williston Basin in Montana and North Dakota. The total area of the Bakken shale oil play and Williston-Shallow Niobraran is 6522 sq. miles.

[d] The gas EUR of Bakken shale oil play is upgraded from Hughes's report.[2] The gas EUR is 120 MBOE (thousand barrels of oil equivalent), wich equals approximately to 0.75 Bcf. (6,000 cubic feet of gas = 1 barrel of oil on an energy equivalent basis)

[e] It has been reported that Marcellus shale play is a combination of dry gas zone and wet gas zone. Only wet gas zone is considered in the calculation.[4] Besides, the Greater Siltstone and Low Thermal Maturity shale plays located in this region are not considered due to their low EUR.

Table S-2 Summary of well numbers, wet well ratio and average age[1, 3]

Region	Total wells	Sampled wells	Wet wells	Wet wells ratio [a]	Ave. age
Appalachia (AP)	81218	164	-	30.0%[a]	1.13
Gulf Coast (GC)	93552	146	71	48.6%	2.31
Mid-continent (MC)	81752	76	29	38.2%	1.23
Rocky Mountain (RM)	338400	78	78	100%	3.92

[a] As mentioned above, Marcellus shale play is a combination of dry gas zone and wet gas zone, and only the latter is considered in the calculation.[4] The wet well ratio of AP region is assumed to be 30%, which is consistent with the ratio of wet gas zone to total zone. The wet well ratios of others regions are updated from Allen and co-workers.[3, 5]

Table S-3 Normalized production decline characteristics in the Appalachia shale region.

Month	Benchmark[6, 7]	Prediction	*D*	*b*	RE
0	0.345	0.345	a=0.655; $P^{\dagger}$=0.345		0.00
1	1.000	1.000	0.2540	1.5090	0.00
6	0.540	0.540	0.2540	1.5090	0.00
12	0.310	0.352	0.2540	1.5090	0.14
18	0.250	0.272	0.2540	1.5090	0.09
24	0.222	0.226	0.2540	1.5090	0.02
36	0.181	0.174	0.2540	1.5090	0.04
48	0.143	0.144	0.2540	1.5090	0.01
60	0.124	0.124	0.2540	1.5090	0.00
				total	0.03

Table S-4: Normalized production decline characteristics in the Midcontinent shale region.

Month	Benchmark[8, 9]	Prediction	*D*	*b*	RE
0	0.456	0.456	a=0.544; $P^{\dagger}$=0.456		0.00
1	1.000	1.000	0.1022	1.1265	0.00
2	0.891	0.908	0.1022	1.1265	0.02
3	0.825	0.832	0.1022	1.1265	0.01
4	0.766	0.768	0.1022	1.1265	0.00
5	0.705	0.714	0.1022	1.1265	0.01
6	0.661	0.668	0.1022	1.1265	0.01
7	0.633	0.627	0.1022	1.1265	0.01
8	0.600	0.592	0.1022	1.1265	0.01
9	0.571	0.560	0.1022	1.1265	0.01
10	0.534	0.532	0.1022	1.1265	0.01
11	0.509	0.507	0.1022	1.1265	0.01
12	0.486	0.484	0.1022	1.1265	0.01
13	0.457	0.463	0.1022	1.1265	0.01
14	0.438	0.444	0.1022	1.1265	0.01
15	0.416	0.426	0.1022	1.1265	0.01
16	0.401	0.410	0.1022	1.1265	0.01
17	0.389	0.396	0.1022	1.1265	0.01
18	0.378	0.382	0.1022	1.1265	0.01
19	0.363	0.369	0.1022	1.1265	0.01
20	0.354	0.357	0.1022	1.1265	0.01
21	0.339	0.346	0.1022	1.1265	0.01
22	0.331	0.336	0.1022	1.1265	0.01
23	0.318	0.326	0.1022	1.1265	0.01
24	0.315	0.317	0.1022	1.1265	0.01
25	0.293	0.308	0.1022	1.1265	0.01
				total	0.01

Table S-5: Normalized production decline characteristics in the Gulf Coast shale region.

Month	Benchmark[8, 9]	Prediction	*D*	*b*	RE
0	0.472	0.472	a=0.528; $P^{\dagger}$=0.472		0.00
1	1	1	0.2522	1.2065	0.00
2	0.837	0.802	0.2522	1.2065	0.04
3	0.699	0.674	0.2522	1.2065	0.04
4	0.586	0.584	0.2522	1.2065	0.00
5	0.516	0.517	0.2522	1.2065	0.00
6	0.465	0.465	0.2522	1.2065	0.00
7	0.414	0.423	0.2522	1.2065	0.02
8	0.379	0.388	0.2522	1.2065	0.02
9	0.348	0.360	0.2522	1.2065	0.02
10	0.324	0.335	0.2522	1.2065	0.02
11	0.295	0.314	0.2522	1.2065	0.02
12	0.27	0.296	0.2522	1.2065	0.01
13	0.258	0.280	0.2522	1.2065	0.01
14	0.243	0.265	0.2522	1.2065	0.02
15	0.226	0.253	0.2522	1.2065	0.02
16	0.218	0.241	0.2522	1.2065	0.02
17	0.207	0.231	0.2522	1.2065	0.02
18	0.197	0.221	0.2522	1.2065	0.02
19	0.182	0.213	0.2522	1.2065	0.02
20	0.175	0.205	0.2522	1.2065	0.02
21	0.171	0.197	0.2522	1.2065	0.02
22	0.162	0.191	0.2522	1.2065	0.02
23	0.156	0.184	0.2522	1.2065	0.02
24	0.147	0.178	0.2522	1.2065	0.02
25	0.132	0.173	0.2522	1.2065	0.02
				total	0.02

Table S-6: Normalized production decline characteristics in the Rocky Mountains shale region.

Month	Benchmark[10, 11]	Prediction	D	b	RE
0	0.530	0.530	a=0.470; $P^{\dagger}$=0.530		0
1	1.000	1.000	0.2994	1.4438	0.00
6	0.450	0.451	0.2994	1.4438	0.00
12	0.310	0.298	0.2994	1.4438	0.04
18	0.230	0.230	0.2994	1.4438	0.00
24	0.190	0.191	0.2994	1.4438	0.00
36	0.160	0.146	0.2994	1.4438	0.09
48	0.122	0.120	0.2994	1.4438	0.02
60	0.095	0.103	0.2994	1.4438	0.09
				total	0.03

1.2 Shale gas composition

Table S-7 Composition of impurity-free shale gas (Mg)[3]

Well-Site [a]	C_1	C_2	C_3	C_4	C_{5+}
AP-w1	52251.344	19068.912	9264.112	4463.62	2701.4928
AP-w2	151073.984	8369.8828	647.5948	56.744	0
AP-w3	203203.552	15549.496	1638.644	309.219	0
GC-w1	9123.760	3150.540	2051.125	1190.330	874.250
GC-w2	177853.376	70371.796	51587.359	33271.3	23357.143
GC-w3	452126.912	169009.946	109086.69	77113	47396.286
GC-w4	125473.648	46750.76	31380.776	21499.6	16396.184
GC-w5	249432.176	75723.9	38708.257	24314.9	15650.992
GC-w6	704633.696	213322.979	109616.79	68609.1	44162.16
GC-w7	211792.064	91544.992	68210.912	47696.4	61543.68
GC-w8	132546.096	43960.548	25772.417	12113.8	7235.789
GC-w9	142965.024	54711.168	37984.456	28522.1	22304.04
GC-w10	6406.928	446.9353	134.9725	85.1365	128.3277
GC-w11	743014.848	202487.351	101862.793	71652.5	55385.473
GC-w12	21829.056	1301.208	387.324	246.384	404.028
GC-w13	234832.272	60240.856	31237.492	18458.5	13325.084
GC-w14	282438.192	110317.254	76602.486	54271.9	58229.196
GC-w15	6257.776	381.943	158.6412	140.062	405.1782
GC-w16	4578.4	507.3316	193.158	126.932	232.578
GC-w17	71813.856	9058.092	3088.182	1749.53	3605.088
GC-w18	13046.08	960.652	350.721	251.37	406.98
GC-w19	11705.6	861.944	314.682	225.54	365.16
GC-w20	15885.632	1113.83	374.986	294.134	553.418
GC-w21	100380.24	23991.603	11238.033	6238.91	4479.216
MC-w1	31278.496	8401.094	8486.696	4401.35	3114.798
MC-w2	235150.4	18578.336	2487.552	638.419	113.3568

MC-w3	499.376	131.5632	92.6464	44.4928	42.24
MC-w4	63048.816	12883.734	10128.24	4726.51	4135.698
MC-w5	14118.464	4037.901	3808.959	2035.64	1437.541
MC-w6	9695.824	2354.551	1575.34	801.905	593.125
MC-w7	40263.488	9047.104	6260.524	2895.04	2297.938
MC-w8	75521.888	17502.026	12772.861	5585.9	4162.743
MC-w9	23587.728	5158.716	3640.611	1858.12	1534.026
RM-w1	17877.472	5492.614	3320.796	2183.36	3137.76
RM-w2	4818.176	1465.684	1012.77	716.1	501.27
RM-w3	16952.352	4816.838	2819.84	1971.69	2423.3
RM-w4	15704.384	4824.692	2916.936	1917.83	2756.16
RM-w5	6897.808	2119.108	1281.176	842.348	1210.56
RM-w6	7983.408	1765.484	750.952	429.57	709.586
RM-w7	8363.84	2569.484	1553.464	1021.37	1467.84
RM-w8	10576.576	3249.589	1964.69	1291.75	1856.4
RM-w9	15038.864	4620.458	2793.492	1836.67	2639.52
RM-w10	11967.088	3821.779	2356.013	1624.28	948.838
RM-w11	2764.032	849.087	513.334	337.507	485.04
RM-w12	16096.144	5572.196	2942.212	1503.32	1675.128
RM-w13	25958.112	7975.125	4821.682	3170.16	4555.92
RM-w14	44000.784	16390.441	12998.66	9090.84	5265.28
RM-w15	2069.248	635.659	384.302	252.671	363.12
RM-w16	97288.64	37111.47	27867.287	16263	9317.33
RM-w17	12636.384	3882.315	2347.214	1543.25	2217.84
RM-w18	26532.064	7538.976	4413.44	3085.96	3792.8

[a] AP: Appalachian, GC: Gulf Coast, MC: Mid Continent, RM : Rocky Mountain, w: wet well.

Table S-8 Average compositions of impurity-free shale gas (w.t.%)

	C_1	C_2	C_3	C_4	C_{5+}
AP	86.75	9.17	2.46	1.03	0.58
GC	57.71	18.32	10.87	7.26	5.84
MC	74.62	11.82	7.45	3.48	2.64
RM	54.55	18.22	12.24	7.79	7.20

Table S-9 Assumed compositions of impurity associated with raw shale gas (mol%) [a]

	CO_2	H_2S	N_2	H_2O
AP [b]	0.73	0.24	2.54	0.10
GC [c]	4.80	1.60	0.10	0.10
MC [d]	1.00	0.33	0.70	0.10
RM [e]	0.57	0.01	5.21	0.10

[a] Based on the previous analysis,[12] if the water vapor is present in a small amount, it has an ignorable effect on the techno-economic performances. Therefore, for all types of shale gases investigated, the concentration of water vapor is set to 0.10 w.t.% in the raw shale gas. H_2S content is reported typically varying at a very low H_2S/CO_2 molar ratio (0.01~0.5).[13] It is assumed to be 0.33 for the H_2S/CO_2 in this study.

[b] The impurity compositions in the AP shale gas is adopted from Bullin and Krousop[14]. Bullin and Krousop reported four compositions that are characteristics of gases produced from the Marcellus play. This work uses the average impurity compositions of sampled wells 1~4.

[c] Updated from Bullin and Krousop.[14]

[d] Updated from EERC report.[15]

1.3 Average delivery distance and pipeline cost

1.3.1 Well-site to processing facility distance

The average delivery distance ($\overline{d_p}$) of raw shale gas from the well-site to a processing facility is equal to the average distance from a random point in the square to the center of the square, see Eq. (S1).

$$\overline{d_p} = \Re\sqrt{\frac{q_p}{Y_g f}}\int_{-0.5}^{0.5}\int_{-0.5}^{0.5}\sqrt{x^2+y^2}\,dxdy = 0.383\times\Re\sqrt{\frac{q_p}{Y_g f}} \tag{S1}$$

where $\Re$ is terrain factor ($\Re \geq 1$, assumed to be 1.2 on average[27,28]), which is a function of a region's pipeline network development and reflects the ratio of actual distance to the ideal straight line distance to a processing facility. q_p, Y_g, and f are the capacity of the processing facility, gas extraction per square mile, and the ratio of wet wells to total wells (or called wet well density, see Fig. 3b) , respectively.

1.3.2 Processing facility to olefins production plant distance

An empirical formula[27] (see Eq. S2) is employed to calculate the average distance that NGLs moved from distributed processing facility to the centralized olefins production plant ($\overline{d_c}$) by pipeline.

$$\overline{d_c} = \Re\phi\sqrt{\frac{q_c}{Y_{NGL} f}}\left(\frac{q_p}{q_c}\right)^{\delta} \tag{S2}$$

where q_c and Y_{NGL} represent the capacity of the olefins production plant and NGLs extraction per square mile; ϕ and δ are empirical coefficients. The distances $\overline{d_p}$ and $\overline{d_c}$ can be further used to estimate the total pipeline lengths of shale gas shipped to the processing facility, and NGLs shipped to the olefins production plant.

1.3.3 Pipeline transportation cost

Table S-10 Pipeline transportation cost estimation models

Cost type	Unit	Economic Model [a 50]	
		Shale gas gathering line	NGLs gathering line [c]
Material	$	$[330.5\times(D)^2+687\times D+26960]L+35000$	0.8×Shale gas_ Material
Labor	$	$[343\times(D)^2+2074\times D+170013]L+185000$	1.0×Shale gas_ Labor
Right of Way	$	$[576.8\times D+29788]L+40000$	0
Miscellaneous	$	$[8417\times D+7324]L+95000$	1.0×Shale gas_Mis.
Capital Cost	$	$[674\times(D)^2+11755\times D+234085]L+355000$	$[607\times(D)^2+11041\times D+198905]L+308000$
Length [b]	mile	$L_p=\Omega_p\times\lambda_p\times N_p\times\overline{d_p}$	$L_c=\Omega_c\times\lambda_c\times N_c\times\overline{d_c}$
O&M[51]	$/year	3%×total capital cost	3%×total capital cost

[a] The units on pipeline diameter (D) and length (L) are inch and mile. The sizing of shale gas pipe and NGLs pipe are given by Tables S-11 and S-12 in SI.

[b] The total pipeline length is a function of average distance ($\overline{d_p}$ and $\overline{d_c}$), merging factor (λ_p and λ_c), number of main pipeline (Ω_p and Ω_c), number of plant (N_p and N_c). Merging factor denotes the ratio of total pipeline length and main pipeline length (due to the existence of auxiliary pipeline).[52] In this model, Ω_p and Ω_c are assumed to be 5 and N_p; the influences of λ_p and λ_c on pipeline transportation costs are shown in Fig. 10.

[c] Here we assume that using existing right of ways will cost nothing.[50]

Table S-11 Shale gas transportation pipe sizing[16]

	Pipeline diameter D (inch)
AP	3
GC	6
MC	6
RM	3

Table S-12 NGLs transportation pipe sizing and flow rate range

Pipeline diameter, D (inch)	NGLs flow rate (Mt/year)	
	Lower bond	Upper bound
5		0.19
7	0.19	0.54
9	0.54	1.13
14	1.13	3.25
19	3.25	6.86
23	6.86	12.26
28	12.26	19.69

2 Plant modeling and integration

Table S-13 General assumptions and default operating conditions used in process simulation

Process Units	Technology	Brief Description	Conditions	Unit	Default
gas Sweetening	scavenger	inlet H_2S mol%<500 ppm	efficiency	%	99.9
	AGR+ scavenger	inlet H_2S mol%>500 ppm	DEA conc.	g/g	0.40
	AGR+ sulfur	H_2S removal>1 Mlb per day	DEA conc.	g/g	0.40
Dehydration	TEG absorption	H_2O w.t.%<0.5	TEG conc.	g/g	1.0
Sulfur removal	AGE+ Claus/SCOT	AGE increases the H_2S mol% from ~30 to ~75;	MDEA conc.	g/g	0.50
			H_2S recovery	%	99.5
NGLs recovery	turbo-expander	outlet N_2 mol%<4, otherwise the N_2 rejection is needed	ethane recovery	%	~80
			Demethanizer top	ºC	-98
N_2 rejection	single distillation integrated with refrigerant cycle	increasing the N_2 mol% from >4 to ~2; the refrigerant	Rejector top	ºC	-127
			refrigerant ratio	mol/mol	0.50
			refrigerant press.	bar	1.1/40
NGLs fractionation	cryogenic distillation	debutanizer co-process C_{4+} from the olefins separation	butanes recovery	%	99.0
			pentanes recovery	%	90.0
Olefins separation	cryogenic distillation; C_2H_2	Separating ethylene and propene from cracking gas; providing pure H_2 or fuel for steam cracking	C_2H_2 conversion	%	99.9
			ethylene recovery	%	99.5
	PSA+ cold-box		propene recovery	%	99.0
			H_2 recovery	%	85.0
Mixture cracking	steam cracking	breaking the mixture C_2+C_3; maximum capacity for a single cracker= 400 ton/hr[17]; the furnace outlet temp. <1500 ºC	steam dilution	kg/kg	0.40
			C_2/C_3 conversion	%	~60/80
			cracker press. drop	bar	2.2
			cracker volume[18]	m^3	6.5
			Heat losses	%	5
Utilities facility	process integration; combined heat and power generation; back steam turbine; MED; TDS removal	energy and water savings; the CHP use back steam turbine to recover sensible heat from the cracking gas; The overall generation efficiency is assumed to be 90%.[19]	temp. approach	ºC	10
			heat transfer coeff.	kW m^2	1.7~5.0
			refrigerant temp.	ºC	-150/-120/-
			steam temp.	ºC	100/300/500
			cold water temp.	ºC	20
			turbine isentropic	%	70

Table S-14 Expressions of reaction rate for ethane-propane mixture[18, 20]

No.	Reaction	Constant of reaction rate [a]	$A_{0,j}$ [1/s or 1/(mol·s)[a]]	$E_{a,j}$ [kJ/mol]	*Base component*
R(1)	$C_3H_8 \rightarrow C_2H_4 + CH_4$	$A_{0,j}EXP(-E_{a,j}/RT)$	$4.692 \cdot 10^{10}$	214.597	propane
R(2)	$C_3H_8 \rightarrow C_3H_6 + H_2$	$A_{0,j}EXP(-E_{a,j}/RT)$	$5.888 \cdot 10^{10}$	214.597	propane
R(3)	$C_3H_8 + C_2H_4 \rightarrow C_2H_6 + C_3H_6$	$A_{0,j}EXP(-E_{a,j}/RT)$	$2.536 \cdot 10^{13}$	247.106	propane
R(4)	$2C_3H_6 \rightarrow 3C_2H_4$	$A_{0,j}EXP(-E_{a,j}/RT)$	$1.534 \cdot 10^{11}$	233.466	propane
R(5) [a]	$6C_3H_6 \rightarrow 5Char + 3CH_4 + 2C_5H_{12}$	$A_{0,j}EXP(-E_{a,j}/RT)$	$7.120 \cdot 10^{8}$	190.371	propane
R(6)	$C_3H_6 \rightarrow C_2H_2 + CH_4$	$A_{0,j}EXP(-E_{a,j}/RT)$	$3.794 \cdot 10^{11}$	248.487	propane
R(7)	$C_3H_6 + C_2H_6 \rightarrow C_4H_8 + CH_4$	$A_{0,j}EXP(-E_{a,j}/RT)$	$1.000 \cdot 10^{14}$	251.081	
R(8)	$C_2H_6 \rightarrow C_2H_4 + H_2$	$A_{0,j}EXP(-E_{a,j}/RT)$	$4.652 \cdot 10^{13}$	272.796	ethane
R(9)	$C_2H_4 + C_2H_2 \rightarrow C_4H_6$	$A_{0,j}EXP(-E_{a,j}/RT)$	$1.026 \cdot 10^{12}$	172.631	ethane
R(10)	$C_2H_6 + C_2H_4 \rightarrow C_3H_6 + CH_4$	$A_{0,j}EXP(-E_{a,j}/RT)$	$7.083 \cdot 10^{13}$	252.838	ethane

[a] The original reaction is $4C_3H_6 \rightarrow 6CH_4 + C_{5+}$.[18] In the new R(5), pentane (C_5H_{12}) represents C_{5+} hydrocarbons. Char is also considered in the equation in consistent with coke formation from propane (C_3H_6).

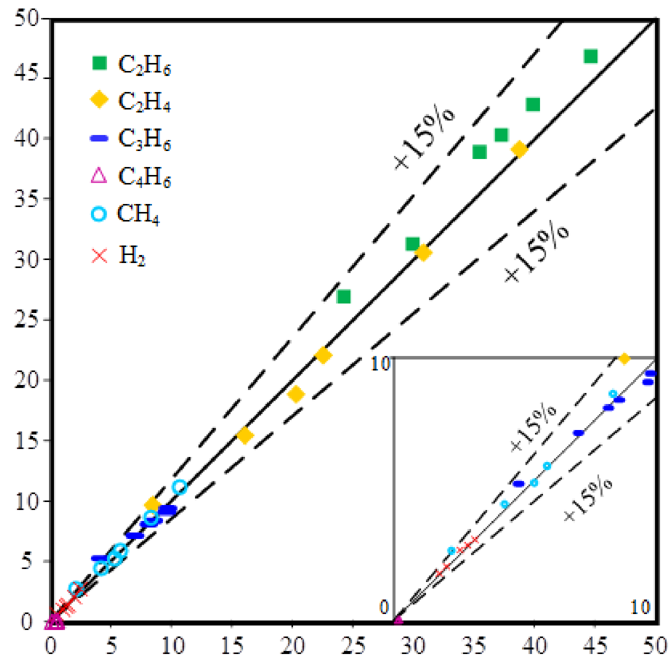

Fig. S-1 Parity plot for cracking gas composition on dry basis

Table S-15 Quality specifications for process water and boiler feed water

Quality specification[21, 22]	Process water	Boiler feed water
hydrocarbon matter [mg/L]	1.0	1.0
TDS [mg/L]	500	2.0
oxygenated compounds [mg/L]	10	10

Table S-16 coefficients used in the calculation of environmental metrics

Coefficient	value/equation
Coefficient of performance (*COP*)	$COP = T_{refri}/(T_{refri} - T_0)$; T_{refri} and T_0 are the temperatures of refrigerant and ambient.[23]
Thermal efficiency of the power cycle (η)	33% (HHV basis)[24]
Emission factor (θ)	
Work (θ_w) and electricity (θ_e)	89.4 kg CO_2-eq/GJ LHV (IPCC[25])
Refrigerant (θ_r)	$\theta_r = q_r/COP \times \theta_e$; q_r is the energy flow of refrigerant.
Heat (θ_h)	56.9 kg CO_2-eq /GJ LHV (based on natural gas power plant)[26]

3 Process yield and consumption

Table S-17 The energy usage in the stage of shale gas production[27]

	Energy consumed (GJ)
Pad preparation	400
Well drilling	27,500
Well cementation	50
Hydraulic fracturing and well completion	6,200
Upstream manufacturing	24,920
Cement and lime	700
Waterproof fabric	50
Casing	6650
Bentonite	50
$CaCl_2$	430
Diesel	16,670
Total	59,100

Table S-18 NGLs transportation pipe sizing and flow rate range[28, 29]

	Drilling (gallon)	Cement (gallon)	Hydraulic fracturing (gallon)		Mean value (MMgallon)
			Lower bond	Upper bound	
AP	180000	24000	2600000	5800000	4.404
GC	280000	37000	3400000	8800000	6.417
MC	170000	19000	3700000	6700000	5.389
RM	-	-	-	-	2.300

Table S-19 GHG emissions related to shale gas production

Item [a]	value
(1) ***Well construction***, kg CO_2eq/well	7.90E+05
sand mining	7.52E+03
sand transport (train)	1.23E+05
sand transport (road)	3.17E+04
casing manufacture	4.95E+05
casing transport (road)	5.16E+03
cement manufacture	9.35E+04
cement transport (road)	1.31E+03
diesel (well to refinery)	2.87E+04
diesel transport to pad (pipeline)	2.65E+02
diesel transport to pad (road),	3.92E+03
(2) ***Well maintenance***, kg CO_2eq/well	8.15 E+05
(3) ***Drilling***, kg CO_2eq/well	3.02E+05
well Drilling	3.01E+05
drilling fugitives	1.16E+03
(4) ***Hydraulic fracturing***, kg CO_2eq/well	2.36 E+05
(5) ***Water-related emissions***,	3.37E+05
wastewater transport, CO_2eq/well	3.15E+05
wastewater injection, CO_2eq/well	6.25E+03
slick water additive manufacture	1.60E+04
(6) ***Additive transport***, kg CO_2eq/well	803
(7) ***Gathering lines***, kg CO_2eq/well/hr	-
Reciprocating Compressors	20.44
Compressor Blowdowns	0.79
Compressor Starts	1.76
Gas Engines	120.30
pipeline leak [b]	-

	AP	GC	MC	RM
(8) ***Pneumatic devices***, kg CO_2eq/well [c]	1.71E+06	3.24E+06	3.50E+06	1.24E+06
(9) ***Pneumatic pumps***, kg CO_2eq/well [c]	4.84E+05	2.36E+05	1.29E+05	0
(10) ***Equipment leak***, kg CO_2eq/well [c]	7.49E+05	3.36E+05	5.38E+05	1.27E+05

[a] The GHG emissions of items 1-10 are estimated using the study of Laurenzi *et. al*.[24]
[b] The calculation of pipeline leak updated from EPA's report[30] are given as follows.
[C] The GHG emissions related to pneumatic devices, pneumatic pump, and equipment leak are taken from refs 3, 5.

Note that the pipeline leak in Table S-19 can be calculated as follows.

(1) Methane leakage from NGLs pipeline. NGLs pipeline is used to transport NGLs (ethane + propane >99 v%, due to pipeline specifications) to steam cracking facilities. Thus, there is no methane leakage.

(2) Methane leakage from gas pipeline. Gas pipeline is used to transport raw shale gas to gas processing facilities, potentially leading to methane leakage due to methane is the major component. According to EPA's report[30], the original data of such leakage is 71.8 scf gas/day/mile, as shown in Fig. S-2.

	Marcellus Activity Factor	EPA Emission Factor
Heaters	1 heater/well	18 scf gas/day/heater
Separators	1 separator/well	1.1 scf gas/day/separator
Meters	1 meter/well	11 scf gas/day/meter
Reciprocating Compressor	†	340 scf gas/day/compressor
Pipeline Leak	0.670 miles/well	71.8 scf gas/day/mile
Pneumatic Device Vents*	2 devices/well	183 scf gas/day/device
Chemical Injection Pumps	1 pump/well	315 scf gas/day/pump
Compressor Exhaust Methane	†	0.30 scf gas emitted/hphr
Vessel Blowdowns	2 vessels/well	99 scf gas/vessel/year
Pipeline Blowdowns	0.670 miles/well	392 scf gas/mile/year
Compressor Blowdowns	†	4789 scf gas/compressor/year
Compressor Start Blowdowns	†	10,714 scf gas/compressor/year
PRV	2 PRV/well	43 scf gas/PRV/year
Mishaps	0.670 miles/well	849 scf gas/mile

Table S4 Key Emission Factors utilized in the production stage of the Marcellus gas LCA[4]

Fig. S-2 Basic emission factors related to shale gas production [24,30]

The amount of methane leakage from gas pipeline can be obtained via the equation below:

Methane Leakage (kmol /hr)=emission factor (scf gas/day/mile)×volume factor (kmol/scf)× pipeline distance (mile)× methane concentration (mol%)÷24 (hr)

Table S-20 lists examples of methane leakage calculation. The equivalent CO_2 emissions associated with pipeline leakage are 83, 8, 25, and 13 kmol CO_2-eq/hr, accounting for 1.87%, 0.16%, 1.70%, and 0.30% of those in the production stage of Appalachian, Gulf Coast, Mid-Continent, and Rocky Mountain shale gases, respectively. When the equivalent CO_2 emissions from olefins production stage are further taken into account, these shares will be correspondingly decreased to 0.30%, 0.10%, 0.30%, and 0.05% according to the normalized GHG emissions of olefins production, respectively, as provided in Fig.12c and Table 5.

Table S-20 Methane leakage calculation

	emission factor	volume factor	pipeline distance [a]	C_1 concentration
AP	71.8	1.203E-03	1,022	89.82%
GC	71.8	1.198E-03	120	72.06%
MC	71.8	1.197E-03	331	85.57%
RM	71.8	1.198E-03	200	70.69%
	C_1 leakage	equivalent CO_2 emissions [b]	total equivalent CO_2 emissions in upstream stage	share, %
AP	3.30	83	4,404	1.87%
GC	0.31	8	4,728	0.16%
MC	1.02	25	1,494	1.70%
RM	0.51	13	4,258	0.30%

[a] pipeline distance is determined under NT+10 yr LT scenario.

[b] based on 100-year global warming potentials (25 kg CO_2-eq/kg CH_4).

4 Economic Evaluations

The indirect plant expenses (*IPE*, e.g., contingency, engineering, and supervision) along with *TDC* give an estimate of the total plant capital cost (*TPC*) required for the process. The products are assumed to be sold from the plant gate and do not include the transportation cost to end-users. All capital costs and market prices of raw feedstocks, products, and utilities involved in the economic evaluation are listed in Table S-18. These prices were converted to 2012 dollars using the Chemical Engineering Plant Cost Index. The *TPC* cost can be converted to total annualized cost (*TAC*) by multiplying a capital recovery factor (*CCF*), as given by Eq. (S-1).

$$TAC = TPC \times CCF + AOC + AFC = TPC \times r(r+1)^N \big/ [(1+r)^N - 1] + AOC + AFC \qquad \text{(S-1)}$$

$$NPV = -TPC + \sum_{t \in T_{ls}} (Rev - TAC)(1 - R_{tax}) / (1+r)^t \qquad \text{(S-2)}$$

where *CCF* is determined as a function of the interest rate (*IR*) and depreciation time of the project (N_{dp}); *AFC* and *AOC* denote the annual raw material cost and annual operating and maintenance cost. The revenue (*Rev*) of this process comes from selling ethylene, propene, pipeline gas, butanes, pentanes, and hydrogen at market price provided in Table 3. In this work, net present value (*NPV*) is used as the economic measurement. To calculate the *NPV*, an economic feasibility study is performed through discounted cash flow analysis following standard procedure,[31] as given by Eq. (S-2). Note that, we also present the break-even shale gas price (BEGP) in $ per MMbtu as the shale gas price for which the *NPV* of the process design is equal to zero. High BEGP is significantly important to reduce the economic risk of shale gas project.

Monte Carlo simulation method, implemented within a spreadsheet based application suite, Oracle Crystal Ball. During the Monte Carlo simulation, the uncertain input is called an “assumption”, and the resulting output is called a “forecast”. In this study, the project economic indicator, *NPV*, is used as the forecast for all case studies. Meanwhile, we specify fifteen assumptions that include raw material, products, electricity and refrigerants prices, as listed in Table S-18. Each selected assumption is assigned a range of values and a uniform distribution based on market values in recent years. Besides, the triangular distributions of *TPC* ranging from ±25% of the deterministic values listed in Table S-19 are assumed in this model.

Table S-21 Capital cost distribution ($MM)

	AP	**GC**	**MC**	**RM**
Sweetening	27.6	21.2	18.0	19.5
AGE+Claus/SCOT	165.3	134.8	75.0	31.1
Dehydration	27.3	12.7	13.7	6.2
NGL recovery	82.4	25.3	43.2	26.2
Compression station	94.2	22.9	44.4	129.0
N_2 rejection	0.0	0.0	0.0	12.4
Fractionation	24.7	36.2	31.6	37.6
Cracking	765.6	775.5	764.4	774.2
Olefins separation	119.4	122.9	119.9	122.3
Utilities unit	39.6	38.8	38.2	38.8
Transportation				
near-term	361.0	50.7	135.8	73.0
mid-term	458.2	87.9	174.5	93.9

TPC×CCF

near-term	466.8	354.1	360.7	361.0
mid-term	488.0	362.3	369.1	365.5
AFC	5,483.2	1,101.7	1,421.4	1,572.3
AOC	96.2	49.4	56.6	61.3
TAC				
near-term	6,046.2	1,505.2	1,838.7	1,994.6
mid-term	6,067.4	1,513.3	1,847.1	1,999.2

Table S-22 Cost parameters and assumptions for process economic evaluation

Items	Base values	Assumptions	Items	Base values	Assumptions
Shale gas	See Table 1	Uniform (-20%, +20%)	Refrigerant	$ 8.34 /MMbtu	Uniform (7.0, 10.0)
Pipeline gas	$ 5.00 /MMbtu	Uniform (3.0, 7.0)	Cooling/boiling water	$ 0.03/ton	Uniform (0.01, 0.06)
Ethane	$ 0.50 /gal	Uniform (0.2, 0.8)	Solvent (DEA, MDEA, TEG)	$ 2700 /ton	Uniform (2200, 3200)
Ethylene	$ 1200 /ton	Uniform (900, 1500)	Low pressure steam (LPS)	$ 10.5/ton	Uniform (7.0, 13.0)
Propane	$ 1.00 /gal	Uniform (0.5, 1.5)	Middle pressure steam (MPS)	$ 12 /ton	Uniform (10.0, 14.0)
Butanes	$ 1.60 /gal	Uniform (1.0,2.2)	Interest rate (IR)	0.03	-
Pentanes+	$ 2.20 /gal	Uniform (1.5, 3.5)	Discounted annual rate (r)	15%	-
Propylene	$ 1340 /ton	Uniform (800,1800)	Tax rate (R_{tax})	30%	-
Sulfur	$ 200/ton	Uniform (100, 300)	Plant life span (T_{ls})	20 years	-
			Project depreciation time (T_{dp})	6 years	-
Electricity	$ 0.07/kwh	Uniform (0.04, 0.1)	Operating time	8000 hr/year	-

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