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Addition/Correction

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Corrections and Additions to "Shale Gas Processing Integrated with Ethylene Production: Novel Process Designs, Exergy Analysis, and Techno-Economic Analysis"

Chang He[†,‡] and Fengqi You*[,†]

[†]Department of Chemical and Biological Engineering, Northwestern University, Evanston, Illinois 60208, United States

[‡]Department of Chemical Engineering, China University of Petroleum, Changping, Beijing 102249, People's Republic of China

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In the original paper,[1] the kinetic model and referenced plant data were taken from a recent paper from Yancheshmeh et al.[2] Yancheshmeh's work[2] mainly follow Sundaram's model.[3] We note that there are some mistakes in side reactions R3, R4, and R5 (shown in Table A2).

As a result of these changes, the predicted byproducts change significantly. However, as pointed out by Froment et al.,[4] the side reactions are much less important in this model, and the resulting byproducts take up a very small proportion. The predicted main products (C_2H_4, H_2, and C_2H_6) have small variations. For example, C_2H_4 is a desired product, which only decreases by 0.53 mol % after a single pass through the cracking reactor. As a result, Figures 12 and 13, as well as a new

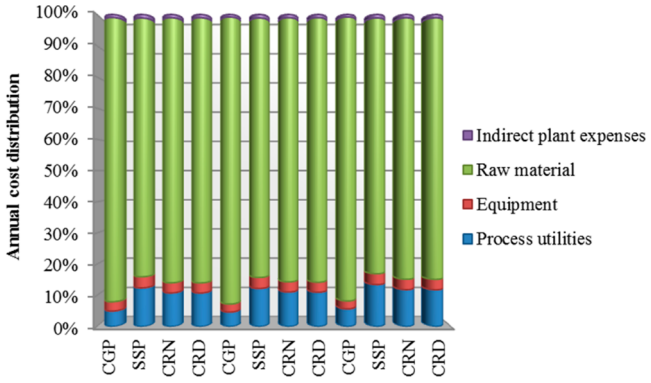

Figure 12. Breakdown of the total annualized cost.

version of Figure 15D and revised versions of Tables 1, 2, 4, and 5, have been revised. These revised figures and tables, as well as a revised version of Table A2, are shown in this Addition/Correction.

- Page 11445: The sentence "The H_2S and CO_2 concentrations are reduced to lower than 4 and 100 ppm, respectively." at the end of the caption for Figure 3 should be deleted.
- Page 11446: The last sentence in section 3.1 needs to be revised. It should read as follows: "After the AGR process, the H_2S and CO_2 concentrations are reduced to 4 ppm and 0.05 mol % in sweet gas, respectively."
- Page 11450: In both Tables 1 and 2, the term "SEP" should be revised to "SSP". In addition, several values have been revised

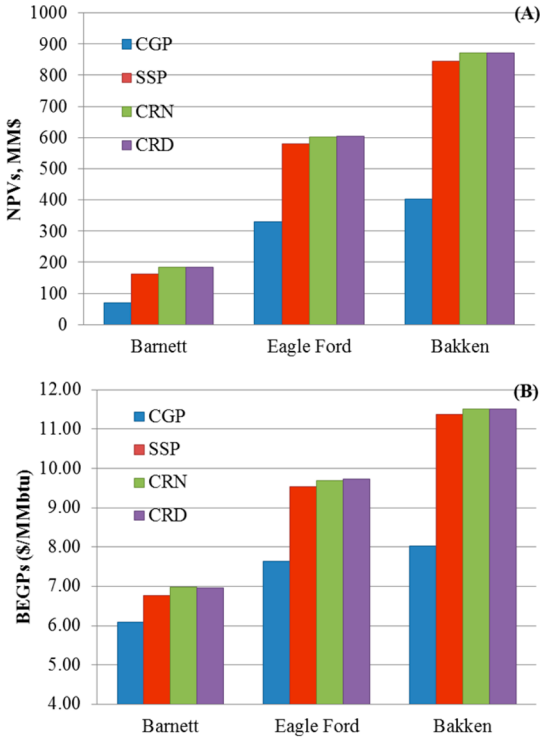

Figure 13. Economic performance results: (A) NPVs and (B) BEGPs.

in Table 1; these values are highlighted in bold font in this Addition/Correction.

- Page 11455: Figure 15D is incorrect; the trend in GHG emissions is not represented correctly. The revised figure is provided in this Addition/Correction. (The top figure is the published figure; the bottom figure is the revised figure.)
- Page 11456: The published version of Table A2 contains some editing errors and mistakes in the kinetic equations. In addition, the 1977 work of Sundaram and Froment (ref 34 in the original paper) and the 2013 work of Shokrollahi Yancheshmeh et al. (published in *Chem. Eng. J.*) each should have been cited as data sources in this table. The corrected table appears in this Addition/Correction.

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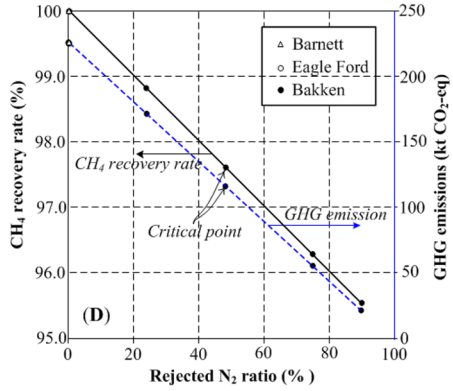
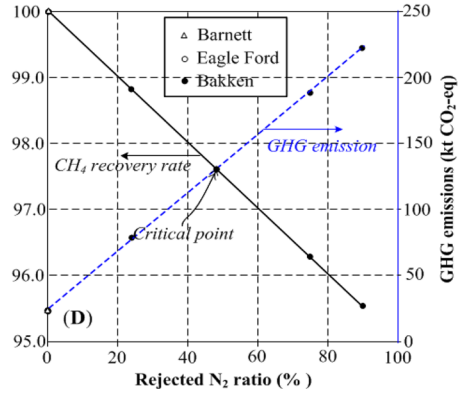
Original:



Revision:



Revised version of Figure 15D.

Table 1. Overall Material Balance for the 12 Case Studies[a]

shale gas type	Barnett				Eagle Ford				Bakken			
design	CGP	**SSP**	CRN	CRD	CGP	**SSP**	CRN	CRD	CGP	**SSP**	CRN	CRD
Inputs												
shale gas (kBD)	17.01	17.01	17.01	17.01	18.78	18.78	18.78	18.78	19.66	19.66	19.66	19.66
Outputs												
sales gas (**MMscfd**[b])	**34.54**	**35.02**	**35.07**	**35.07**	**30.39**	**31.02**	**31.52**	**31.53**	**23.23**	**24.16**	**24.36**	**24.37**
ethane (kBD)	**1.535**	0	0	0	**3.218**	0	0	0	**4.700**	0	0	0
ethylene (ton/day)	0	**65.01**	**64.53**	**64.53**	0	**140.14**	**137.84**	**137.82**	0	**206.24**	**204.54**	**204.51**
hydrogen (ton/day[c])	0	**3.63**	**3.62**	**3.62**	0	**8.91**	**8.90**	**8.90**	0	**13.46**	**13.39**	**13.40**
propane (kBD)	**0.479**	**0.518**	**0.518**	**0.518**	**1.417**	**1.470**	**1.470**	**1.470**	2.950	**3.030**	**3.031**	**3.030**
propene (ton/day)	0	0.011	0	0	0	0.027	0	0	0	0.031	0	0
butanes (kBD)	0.392	**0.405**	**0.406**	**0.405**	0.815	0.843	0.845	0.846	**1.104**	**1.214**	**1.215**	**1.215**
pentanes (kBD)	**0.115**	0.119	**0.118**	**0.118**	**0.771**	**0.775**	**0.775**	**0.775**	**0.495**	**0.497**	**0.497**	**0.496**
sulfur (ton/day)	11.20	11.20	11.20	11.20	12.30	12.30	12.30	12.30	0	0	0	0

[a]Corrections are given in boldface. [b]MMscfd = millions of standard cubic feet per day. [c]In the original paper, the units were MMmol/day.

Table 2. Exergy Efficiency of the Shale Gas-Based Process Designs (btu/s)

shale gas type	Barnett				Eagle Ford				Bakken			
design	CGP	**SSP**	CRN	CRD	CGP	**SSP**	CRN	CRD	CGP	**SSP**	CRN	CRD
Inputs												
feedstock	470401	470401	470401	470401	576407	576407	576407	576407	619206	619206	619206	619206
process utilities												
(u1)heat	**2478**	**8668**	**7918**	**7824**	**3189**	**9737**	**7922**	**7601**	**3383**	**11079**	**9658**	**9480**
(u2)cold	**2362**	**3508**	**2654**	**2553**	**2755**	**4224**	**3164**	**3065**	**2985**	**4816**	**3574**	**3385**
(u3)electricity	**7017**	**19029**	**16125**	**16242**	**7664**	**22978**	**20623**	**20608**	**10435**	**27692**	**24272**	**24262**
(u4)waters	323	413	393	393	383	473	469	469	403	483	476	476
(u5)solvents	56	56	56	56	80	80	80	80	96	96	96	96
Outputs												
sales gas	**379049**	**384372**	**384921**	**384921**	**333554**	**340469**	**345957**	**346067**	**255103**	**265190**	**267454**	**267526**
ethane	**45910**	**0**	**0**	**0**	**96456**	**0**	**0**	**0**	**140878**	**0**	**0**	**0**
ethylene	**0**	**34515**	**34260**	**34260**	**0**	**74403**	**73182**	**73171**	**0**	**109496**	**108594**	**108578**
propane	**20668**	**22351**	**22351**	**22351**	**61141**	**63428**	**63428**	**63428**	**127286**	**130738**	**130825**	**130738**
butanes	**17905**	**18499**	**18752**	**18705**	**37642**	**38935**	**39027**	**39073**	**50989**	**56070**	**56116**	**56116**
pentanes	**6099**	**6311**	**6258**	**6258**	**40890**	**41102**	**41102**	**41102**	**26252**	**26358**	**26358**	**26305**
hydrogen	**0**	**4637**	**4624**	**4624**	**0**	**11381**	**11368**	**11368**	**0**	**17192**	**17103**	**17116**
Byproducts												
(p1)propylene	0	**195**	0	0	0	511	0	0	0	580	0	0
(p2)sulfur	725	725	725	725	800	800	800	800		0	0	0
(p3)heat	268	328	322	320	551	521	502	510	502	789	760	765
overall exergy efficiency (%)	**97.51**	**94.00**	**94.91**	**94.91**	**96.71**	**93.10**	**94.53**	**94.62**	**94.42**	**91.41**	**92.38**	**92.42**

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Table 4. Feedstocks/Products and Process Utilities Cost Distributions (MM$/yr)

shale gas type	Barnett				Eagle Ford				Bakken			
design	CGP	SSP	CRN	CRD	CGP	SSP	CRN	CRD	CGP	SSP	CRN	CRD
Raw material												
shale gas	75.87	75.87	75.87	75.87	92.80	92.80	92.80	92.80	99.87	99.87	99.87	99.87
Process utilities												
(u1)heat	0.10	**0.35**	**0.32**	**0.31**	**0.13**	**0.39**	**0.32**	**0.31**	**0.14**	**0.45**	**0.39**	**0.38**
(u2)cold	0.57	**0.82**	**0.64**	**0.62**	**0.66**	**1.01**	**0.76**	**0.74**	**0.72**	**1.16**	**0.86**	**0.81**
(u3)electricity	4.15	**11.30**	**9.59**	**9.58**	**4.53**	**13.57**	**12.19**	**12.12**	**6.11**	**16.41**	**14.24**	**14.22**
(u4)waters	0.12	0.15	0.15	0.15	0.14	0.17	0.17	0.17	0.15	0.18	0.18	0.18
(u5)solvents	0.02	0.02	0.02	0.02	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03
Outputs												
sales gas	**65.50**	**66.42**	**66.51**	**66.51**	**57.64**	**58.83**	**59.78**	**59.80**	**44.06**	**45.82**	**46.21**	**46.23**
ethane	**10.75**	0	0	0	**22.53**	0	0	0	**32.90**	0	0	0
ethylene	0	**26.00**	**25.81**	**25.81**	0	**56.06**	**55.14**	**55.13**	0	**82.50**	**81.82**	**81.80**
propane	**6.71**	**7.25**	**7.25**	**7.25**	**19.84**	**20.58**	**20.58**	**20.58**	**41.30**	**42.42**	**42.45**	**42.42**
butanes	**8.78**	**9.07**	**9.09**	**9.07**	**18.26**	**18.88**	**18.93**	**18.95**	**24.73**	**27.19**	**27.22**	**27.22**
pentanes	**3.54**	**3.67**	**3.63**	**3.63**	**23.75**	**23.87**	**23.87**	**23.87**	**15.25**	**15.31**	**15.31**	**15.28**
hydrogen	0	**2.13**	**2.12**	**2.12**	0	**5.23**	**5.22**	**5.22**	0	**7.90**	**7.86**	**7.86**
Byproducts												
(p1)propylene	0	0.005	0	0	0	0.012	0	0	0	0.014	0	0
(p2)sulfur	0.750	0.750	0.750	0.750	0.810	0.810	0.810	0.810	0	0	0	0

Table 5. Capital Cost Distribution

shale gas type	Barnett				Eagle Ford				Bakken			
design	CGP	SSP	CRN	CRD	CGP	SSP	CRN	CRD	CGP	SSP	CRN	CRD
Capital cost (MM$)												
total direct cost, TDC	16.15	21.15	18.92	18.78	16.91	25.41	23.12	22.82	18.18	27.69	25.35	25.06
indirect plant expenses, IPE	5.17	6.77	6.05	6.01	5.41	8.13	7.40	7.30	5.82	8.86	8.11	8.02
total plant capital cost, TPC	21.32	27.92	24.97	24.79	22.32	33.54	30.52	30.12	24.00	36.55	33.46	33.08
annual operating cost, AOC	**4.95**	**12.64**	**10.71**	**10.68**	**5.49**	**15.18**	**13.47**	**13.36**	**7.14**	**18.23**	**15.70**	**15.62**
raw material cost	75.87	75.87	75.87	75.87	92.80	92.80	92.80	92.80	99.87	99.87	99.87	99.87
total annualized cost, TAC (MM$/yr)	**80.82**	**88.51**	**86.57**	**86.55**	**98.29**	**107.98**	**106.27**	**106.17**	**107.01**	**118.09**	**115.56**	**115.49**
shale gas processing cost ($/MMbtu shale gas)	**5.97**	**6.53**	**6.39**	**6.39**	**5.93**	**6.52**	**6.41**	**6.41**	**6.00**	**6.62**	**6.48**	**6.48**

Table A2. Expressions of Reaction Rate and Corresponding Model Validation

No.	reaction	constant of reaction rate[a]
R(1)[b,c]	$C_2H_6 \leftrightarrow C_2H_4 + H_2$	$k_1(4.65 \times 10^{13}, 2.73 \times 10^5)\left[\frac{F_{C_2H_6}}{F_t}\cdot\frac{P_t}{RT} - \frac{F_{C_2H_4}F_{H_2}}{F_t^2 K_{C1}}\left(\frac{P_t}{RT}\right)^2\right]$
R(2)[b]	$2C_2H_6 \rightarrow C_3H_8 + CH_4$	$k_2(3.85 \times 10^{11}, 2.73 \times 10^5)\left[\frac{F_{C_2H_6}}{F_t}\cdot\frac{P_t}{RT}\right]$
R(3)[b,d]	$C_3H_6 \leftrightarrow C_2H_2 + CH_4$	$k_3(9.81 \times 10^{8}, 1.54 \times 10^5)\left[\frac{F_{C_3H_6}}{F_t}\cdot\frac{P_t}{RT} - \frac{F_{C_2H_2}F_{CH_4}}{F_t^2 K_{C5}}\left(\frac{P_t}{RT}\right)^2\right]$
R(4)[b]	$C_2H_2 + C_2H_4 \rightarrow C_4H_6$	$k_4(1.03 \times 10^{12}, 1.73 \times 10^5)\left[\frac{F_{C_2H_2}F_{C_2H_4}}{F_t^2}\left(\frac{P_t}{RT}\right)^2\right]$
R(5)[b]	$C_2H_6 + C_2H_4 \rightarrow C_3H_6 + CH_4$	$k_5(7.08 \times 10^{13}, 2.53 \times 10^5)\left[\frac{F_{C_2H_6}F_{C_2H_4}}{F_t^2}\left(\frac{P_t}{RT}\right)^2\right]$

basis mol %)	C_2H_4	H_2	C_2H_6	CH_4	C_3H_8	C_3H_6	C_2H_2	1,3-C_4H_6
modeling result	33.54	37.68	20.53	5.22	0.18	0.20	0.26	2.2
plant data[e]	34.56	37.36	20.60	5.81	0.08	0.51	0.27	0.81[f]
relative error, RE	2.95	0.85	0.33	10.32	125.00	62.74	3.70	171.6

[a]Data taken from ref 34. [b]$k_i(A, E_a)$ follows the Arrhenius equation $k_i(A,E_a) = A \times \exp[-E_a/(RT)]$, where A is the Arrhenius constant (given in units of s^{-1} or $mol^{-1}\ s^{-1}$), E_a the activation energy (J mol^{-1}), F the molar flow rate (mol s^{-1}), P_t the total pressure (Pa), T the reaction temperature (K), and R the universal gas constant (given in units of J $(mol\ K)^{-1}$ or Pa m^3 $(mol\ K)^{-1}$. [c]$K_{C1} = 8.895 \times 10^{-3}$ at 775 °C, 1.276×10^{-2} at 800 °C, 1.800×10^{-2} at 825 °C. [d]$K_{C5} = 9.847 \times 10^{-3}$ at 775 °C, 1.375×10^{-2} at 800 °C, 1.890×10^{-2} at 825 °C. [e]Data taken from: Shokrollahi Yancheshmeh, M. S.; Seifzadeh Haghighi, S.; Gholipour, M. R.; Dehghani, O.; Rahimpour, M. R.; Raeissi, S. Modeling of ethane pyrolysis process: A study on effects of steam and carbon dioxide on ethylene and hydrogen productions. *Chem. Eng. J.* **2013**, *215−216*, 550−560. [f]All C_{4+} hydrocarbons are considered to be 1,3-C_4H_6.

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AUTHOR INFORMATION

Corresponding Author

*E-mail: you@northwestern.edu.

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