Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Appendix A

Carbon Capture from Corn Stover Ethanol Production via Mature CBP Enables Large Negative Biorefinery GHG emissions and Fossil Fuel-Competitive Economics

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Appendix A.1. Table 1. Survey of Technoeconomic Studies for Cellulosic Ethanol Production

	Study		Published (Project Year)	Feedstock	Process	Feed Cost ($/dry metric	Ethanol (MGY)	MESP ($)	Notes
NREL/TP-580-26157	Wooley et al.	(1)	1999 (1997)	yellow poplar	DAP	27.5	52.2	1.44	Biomass-to-ethanol
NREL/TP-580-28893	McAloon et al.	(2)	2000 (1999)	corn stover	DAP	38.5	25	1.50	Compares corn starch and stover
NREL/TP-510-32438	Aden et al.	(3)	2002 (2000)	corn stover	DAP	33.1	69.3	1.07	Stover-to-ethanol
NREL/TP-6A2-46588	Kazi et al.	(4)	2010 (2007)	corn stover	DAP	83.0	53.4	3.40	Compares four pretreatments, seven scenarios, and estimates pioneer plant
NREL/TP-5100-47764	Humbird et al.	(5)	2011 (2007)	corn stover	DAP	64.5	61.0	2.15	Stover-to-ethanol update
	Eggeman and	(6)	2005	corn stover	DAP	35.0	56.1	1.34	Compares pretreatments

	Elander								and concludes DAP has best performance
	Sendich et al.	(7)	2008	corn stover	AFEX	40.0	53.8	1.03 (SSCF)	Varies CBP and SSCF, AFEX parameters
	Huang et al.	(8)	2009	corn stover	DAP	63.8	67.4	1.42	Varies biomass type and throughput
	Klien-Marcuschamer et al.	(9)	2010 (2009)	corn stover	DAP	70.5	30.9	4.58	Wiki-based biorefinery platform
	Bals et al.	(10)	2011 (2008)	corn stover	AFEX	50	23	1.86	Optimizes AFEX conditions
	Meyer et al.	(11)	2013 (2007)	corn stover	HW	64.5	47.4	2.51	Varies yeast processes
	Tao et al.	(12)	2013 (2007)	corn stover	DAP	64.5	59.0	2.21	Varies corn stover composition
	Chen et al.	(13)	2015 (2007)	corn stover	DDR	64.5	64	2.24	Varies deacetylation and disk refining (DDR) technique
	Yang and Rosentrater	(14)	2015	corn stover	LMAA	36.3	50	3.86	Low Moisture Anhydrous Ammonia pretreatment
	Zhao et al.	(15)	2015	corn stover	DAP	59.2	60.5	2.86	China specific economic data, compares NREL and Chinese status quo (NREL-CN-1 data shown here)
	Liu and Bao	(16)	2017 (2013)	corn stover	DryPB		60.1	1.79	Dry acid pretreatment and several others
	Lynd et al.	(17)	2017 (2014)	corn stover	CBP	84.5	60.0	1.88	Forecasted C-CBP (reference case for this study)
	Stoklosa et al.	(18)	2017 (2012)	corn stover	AFEX	60		2.09	Centralized v. decentralized corn stover processing depots
	Huang et al.	(19)	2018 (2007)	corn stover	DAP	58.5	38.1	2.16	Modeled to breakeven while coproducing

									1,5-PDO
	Shen, Tao, and Yang	(20)	2018 (2014)	corn stover	DAP	85.0	57.2	2.83	Modeled to breakeven while coproducing jet fuel from lignin
	Yang et al.	(21)	2020 (2019)	sorghum	DAP	95.0		3.40	Concerns RNG and CO_2 capture with onsite solids combustion
	Das et al.	(22)	2022 (2018)	corn stover	DAP	64.5	61.4	2.47	Compares Humbird et al., 2011 model (updated to 2018) to Py-ECH

DAP = Dilute Acid Pretreatment, AFEX = Ammonia Fiber Expansion, DryPB = Dry Acid Pretreatment, LMAA = Low Moisture Anhydrous Ammonia, CBP = Consolidated Bioprocessing, HW = Hot Water, DDR = Deacetylation and Disk Refining. Py-ECH = pyrolysis with electrocatalytic hydrogenation.

Appendix A.2. Table 2. Fermentation Conditions and Assumed Conversions

Fermentation Conditions and Assumed Conversions			
Parameter		**Original**	**Revised**
Temperature (°C)		55	
Initial Solid Loading (wt.%)		19.5% total (59.7% carbohydrates, 23.8% insolubles, 16.5% extractives)	
Residence Time (days)		6	
Corn Steep Liquor (CSL)	Loading (wt.%)	0.155	0.64
Inorganic Nitrogen Loading	Loading (g/L)	0.261 (DAP)	0.387 (urea)
Carbohydrate Solubilization (%)		88	
Solubilized Carbohydrates	Total Conversion (%)	98.06	
	Conversion to Products (%)	85.55	
	Conversion to Cells (%)	4.75	
	Conversion to Byproducts (%)	4.75	
	Losses to Contamination (%)	3	
Ethanol	Titer (g/L)	50.26	
	Productivity (g/L-day)	8.36	
	Annual Production (MGY)	60.03	

Appendix A.3. Table 3. Gas Turbine Performance Parameters

Gas Turbine Conditions and Assumptions				
Parameters		**References**	**This Study**	
			Biogas Turbine	**RNG Turbine**
Scenarios		(this study)	II & III	V
Ambient Conditions	Temperature (°C)	15 (23–25)	25	
	Pressure (bar)	1.013 (23–26)	1.013	
Fuel Conditions	Temperature (°C)	10 (25)	28	
	Pressure (bar)	30 (25)	1.2	20
Inlet	Air Feed Rate (kg/s)	635 (25) 651 (26)	18.1	17.6
	Fuel Feed Rate (kg/s)	14.74 (25) 0.38 (24) 6.0 (23)	0.48	0.46
Compressor	Pressure Ratio	15.4 (25) 15.6 (24) 18 (23) 17 .03 (26)	15.4	
	Mechanical Efficiency (%)	99 (25) 99.5 (24)	99	
	Isentropic Efficiency (%)	88 (23,25) 85.28 (24) 89.5 (26)	88	
Combustor	Combustion Efficiency (%)	99.5 (25) 99 (23) 99.1 (26)	99.5	
Turbine	Inlet Temperature (°C)	1328.0 (25) 1286 (24) 1232 (23) 1480 (26)	1342	1400
	Exhaust Temperature (°C)	615.0 (25) 548.5 (24) 566 (23) 597.4 (26)	675	698
	Exhaust Gas Rate (kg/s)	21.09 (24) 70.5 (23)	18.6	18.1
	Isentropic Efficiency (%)	84.66 (24) 87 (23)	90	

		90 (26)		
Generator	Generator Efficiency (%)	98.5 (25) 98 (24)	98.5	
Performance	Net Power Generation (kWh)	253,200 (25) 6,327 (24) 25,060 (23) 270,494 (26)	8,830	8,922
	Thermal Efficiency (%)	36.17 (25) 33.13 (24) 36.0 (23) 38.2 (26)	37.0	38.6

Appendix A.4. Table 4. Biogas Membrane Upgrading Performance Parameters

Parameters	**Deng & Hägg** (27) **[scaled]**	**This Study**
Raw Biogas Feed (Nm^3/h)	1,000 [13,714]	13,714
Feed pressure (bar)	1.2	1.2
Feed CO_2 concentration (vol.%)	35	47.8
Feed T and P at 1st and 2^{nd} stage (°C, bar)	25, 20	28, 20
Permeate T and P at 1st and 2^{nd} stage (°C, bar)	25, 1	28, 1
CH_4 purity (vol.%)	98	98
CH_4 recovery (%)	99.7	99.7
CO_2 purity (vol.%)	98.1	99.4
Recycle Ratio	0.24	0.23
Compression duty (kWh)	220 [3,017]	3,043
Compressor Isentropic Efficiency (%)	0.75	0.88
Upgraded biomethane delivery pressure (bar)	40	20

Appendix A.5. Table 5. Scenario Results Summary

		Process design parameters												
Scenario		Enhanced heat integration	Biogas surplus to turbine	Fermentation CO_2 to CCS	Biogas membrane upgrade to RNG	RNG surplus to turbine	Additional Inputs			Exports			GHG benefits
Reference case		no	no	no	no	no	17,463	kWh	electricity	7,137	gal/hr	ethanol	fuel pellets displace fossil fuels
							3,028	kg/hr	nutrients	32,278	kg/hr	fuel pellets	
							1,351	kg/hr	natural gas				
I	Enhanced heat integration	yes	no	no	no	no	17,463	kWh	electricity	7,132	gal/hr	ethanol	no longer consumes natural gas
							3,028	kg/hr	nutrients	32,300	kg/hr	fuel pellets	
II	Biogas electricity	yes	yes	no	no	no	8,845	kWh	electricity	7,132	gal/hr	ethanol	Net electricity demand reduced 49%
							3,028	kg/hr	nutrients	32,300	kg/hr	fuel pellets	
III	Biogas electricity and fermentation CO_2 to CCS	yes	yes	yes	no	no	11,746	kWh	electricity	7,132	gal/hr	ethanol	Fermentation CO2 is now captured
							3,028	kg/hr	nutrients	32,300	kg/hr	fuel pellets	
										21,080	kg/hr	CO_2	
IV	RNG and high-purity CCS	yes	no	yes	yes	no	11,746	kWh	electricity	7,132	gal/hr	ethanol	Biogas CO2 is now captured
										32,300	kg/hr	fuel pellets	RNG surplus displaces fossil fuels
							3,028	kg/hr	nutrients	32,907	kg/hr	CO_2	
										830	kg/hr	RNG	
V	RNG electricity and high-purity CCS	yes	no	yes	yes	yes	11,746	kWh	electricity	7,132	gal/hr	ethanol	Net electricity demand reduced 7%
							3,028	kg/hr	nutrients	32,300	kg/hr	fuel pellets	
										32,907	kg/hr	CO_2	

Appendix A.6. Calculations for Levelized Cost of CO_2 Capture

CO_2 (fermentation only)

Equipment Contribution: 1) CO_2 compressor

$$6.68\ MM\$_{CO2\ compressor} \times 0.15_{capital\ charge\ factor} = 1.00\ MM\$_{annualized\ capital\ cost}$$

Electricity Contribution:

$$2{,}841\ kWh_{CO2\ compressor\ demand} \times 0.0681 \frac{\$}{kWh} = 193.47 \frac{\$}{hour}$$

$$193.5 \frac{\$}{hour} \times 8{,}410 \frac{hours}{year} = 1.62\ MM\$_{annual\ electric\ demand}$$

Sum of Contributions:

$$1.00\ MM\$_{annualized\ capital\ cost} + 1.62\ MM\$_{annual\ electric\ demand} = 2.62\ MM\$_{\ annualized\ cost}$$

Annual CO_2 Production: 177,209 ton/year

$$2.12\ MM\$_{annualized\ cost} \div 177{,}209 \frac{ton}{year} = 14.78 \frac{\$}{ton}\ CO_2$$

CO_2 (fermentation & biogas combined)

Equipment Contribution: 1) CO_2 compressor

$$8.68\ MM\$_{CO2\ compressor} \times 0.15_{capital\ charge\ factor} = 1.30\ MM\$_{annualized\ capital\ cost}$$

Electricity Contribution:

$$4{,}364\ kWh_{CO2\ compressor\ demand} \times 0.0681 \frac{\$}{kWh} = 297.18 \frac{\$}{hour}$$

$$297.18 \frac{\$}{hour} \times 8{,}410 \frac{hours}{year} = 2.50\ MM\$_{annual\ electric\ demand}$$

Sum of Contributions:

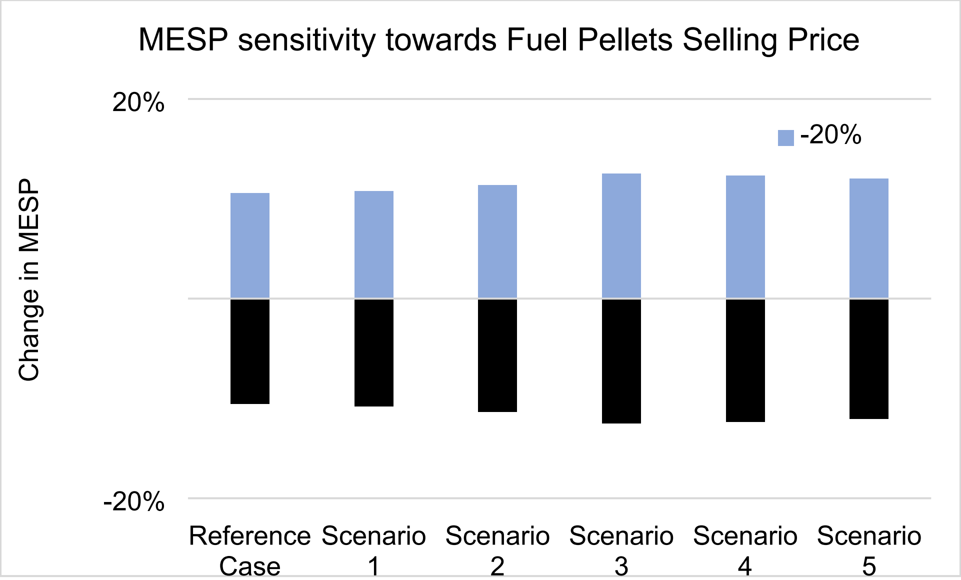
$$1.30\ MM\$_{annualized\ capital\ cost} + 2.50\ MM\$_{annual\ electric\ demand} = 3.80\ MM\$_{\ annualized\ cost}$$

Annual CO_2 Production: 276,659 ton/year

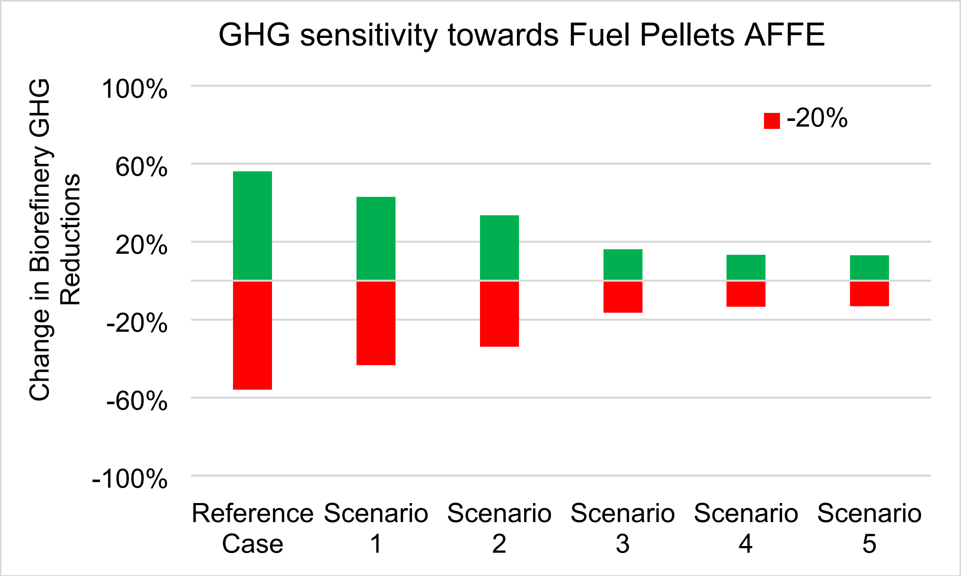
$$3.80\ MM\$_{annualized\ cost} \div 276{,}659 \frac{ton}{year} = 13.74 \frac{\$}{ton}\ CO_2$$

Appendix A.7. Fuel Pellet Production Sensitivity Analysis.

It was observed that increasing or decreasing fuel pellet selling prices has a uniform effect on the MESP related to equal fuel pellet throughput amongst the scenarios. To put it another way, the modifications made to improve the biorefinery GHG balance did not change the MESP's sensitivity towards fuel pellet selling prices. A 20% change (+ or -) in fuel pellet price (baseline $166/ton) did not change the MESP by 20% which is consistent with fuel pellet revenue making up less than half of total revenue in Figure 3.B.



In a second sensitivity analysis, the fuel pellet contribution to avoided fossil fuel emissions (AFFE) in figure 4 are subject to + or – 20%. Since the later scenarios have greater negative carbon flux overall, any perturbation to the fuel pellet AFFE (consistent amongst all scenarios) will be effectively diluted out by the larger contributions enabled by CCS. Thus, later scenarios are less sensitive to the fuel pellet AFFE than those without CCS.



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