Technoeconomic comparison of decentralized biomass pyrolysis and electrocatalysis to cellulosic ethanol for making liquid fuels

Supplementary Information File

1. Equipment Costing & Operating Costs

This section lists and describes the assumptions used for calculating equipment costs for the unit operations within the biomass pyrolysis-electrocatalysis (Py-ECH) depot and the centralized refinery.

1.1. Depot Equipment Costs:

The depot was subdivided into six distinct areas, namely: Drying and Grinding, Pyrolysis, Condensation, Electrocatalytic Hydrogenation, Storage, and Combustion. Most of the purchased equipment costs at the depot were estimated using the online calculator for "Equipment Costs- Plant Design and Economics for Chemical Engineers" by Peters and Timmerhaus.[1, 2]

1.1.1 Drying and Grinding:

Drying equipment cost was calculated for a rotary dryer using the rate of water evaporation needed to reduce biomass moisture content from 20% to 5% by mass.[1, 2] A ball mill was selected to reduce the feedstock from >50 mm to 2 mm particles.[1, 2] The grinding cost is almost twice that assumed by Hess et al.,[3] in terms of 2008$/dry ton/grinding unit. However, the ground size assumed in this study (2 mm) is lesser than that assumed by Hess et al. (38 mm).

1.1.2 Pyrolysis:

The purchased equipment costs for pyrolysis were estimated based on the calculated heat duty of the pyrolysis furnace.[1, 2]

1.1.3 Condensation:

For condensation of the bio-oil after pyrolysis, the heat transfer area was calculated from the heat transfer rate, the log mean temperature difference of the two fluids, and the heat transfer rate coefficient of a shell-and-tube heat exchanger.[4] Using the required heat transfer area, the cost of a shell-and-tube heat exchanger was estimated.[1, 2]

1.1.4 Electrocatalytic Hydrogenation (ECH):

The ECH reactor system has been described in detail in our previous work[5] and previous literature.[6-13] The ECH reactor for this analysis has been assumed to be a collection of polymer electrolyte membrane (PEM) stacks.[7, 11, 14, 15] In these PEM stacks, the catalytic Ru cathode and the Pt anode are pasted on two sides of a Nafion proton exchange membrane. Capital costs for the ECH reactor system are dominated by the costs of the Pt anode, Ru cathode, and the Nafion membrane. The amounts of Pt and Ru required for the ECH reactor were estimated from the current densities, bulk densities, catalyst thickness, and the electricity requirements to chemically reduce the pyrolysis bio-oil. The surface area and costs for the Nafion membrane were determined using the Nafion bulk density, acid capacity, and the electricity requirements. It has been estimated that the membrane and electrode costs are only 60% of the total stack cost; the stack, in turn accounts for only about 40% of the total electrolyser capital cost.[16] The replacement costs were estimated to be about 15% of the installed capital costs, with a replacement schedule of 7 years.[16, 17] This cost was incorporated in the analysis as an annual variable cost. The installation costs were assumed to be 15% of the total uninstalled capital costs.[17] Electricity costs were assumed, in accordance with the Humbird et al. report, at 6.56 ¢/kWh. Similarly, fresh water costs were also assumed from the same report at $ 0.22/tonne in 2007$.[18]

1.1.5 Storage:

Storage costs for H_2 generated from ECH at the depot were calculated by assuming underground storage.[19] Bio-oil storage at the depot occurs in shop-fabricated stainless steel tanks with walls of thickness 6.35 cm.[1] Stainless steel was chosen as the storage material, as only 304L and 316L stainless steel satisfy the criterion for corrosion rates of <0.25 mm/year when in contact with ECH-treated bio-oil.[20] Lu et al., also observed that stainless steel was the most resistant to corrosion from bio-oil when compared to mild steel, aluminum, and brass.[21] Corrosion resistant materials were chosen despite ECH stabilization, which renders bio-oil much less corrosive than pyrolysis bio-oil.

1.1.6 Combustion:

A gas-fired furnace was sized to combust the non-condensable gases (NCG) and a fraction of the H_2 gas to provide heat for all processes at the depot such as pyrolysis.[22]

1.2. Refinery Equipment Costs:

The central refinery was subdivided into three units, namely, the electrolysis unit (used to make hydrogen for hydroprocessing), the storage unit, and the hydroprocessing unit. The raw material for the refinery is the stable bio-oil product delivered from the depots.

1.2.1 Storage:

Storage costs for the final hydroprocessed bio-oil were estimated from fabricated stainless steel tanks with wall thickness equal to 6.35 cm.[1, 2]

1.2.1 Electrolysis:

Electrolyzer capital costs to make H_2 gas for hydroprocessing the stable bio-oil at the refinery can vary over a large range. In 2018, Saba et al. conducted a comprehensive review of the cost of electrolyzers over the past 30 years and found them to range between € 306 (per kW of HHV of H_2 produced in 2017€) and € 37,521 (per kW of HHV of H_2 gas produced in 2017€), depending on electrolyzer type, assumed efficiency, production scale and year of estimation.[23] Based on the values reported by Saba et al., projected electrolyzer costs in 2030 will range from € 397 to € 955 (per kW of HHV of H_2 produced in 2017€). Therefore, for the purposes of this analysis, an average value of € 676 (per kW of HHV of H_2 produced in 2017€) was chosen. This translates to assuming a cost of $ 1,420/(kg/day) produced in 2018$. Stack replacement costs were considered to be 15% of installed capital costs over 7 years as assumed for ECH at the depot. As with ECH electricity supply in depots, electricity costs were assumed to be 6.56 ¢/kWh, in line with the Humbird et al. report.

1.2.2. Hydroprocessing:

Hydroprocessing costs were estimated by scaling-up the costs associated with a hydroprocessing facility that subjects pyrolysis bio-oil to H_2 at elevated temperatures and pressures in the presence of sulfided Co-Mo catalyst, as determined by Dutta et al. in a joint report by NREL and PNNL in 2015 for processing blended woody biomass.[24] In the Dutta report, the hydroprocessing area houses equipment that is very similar to what would be expected in the hydroprocessing section of the central refinery for the Py-ECH system, i.e. a hydrotreater, hydrocracker, compressors, product separation columns, and heat integration facilities. Therefore, when scaled by the amount of hydroprocessor feed, the estimated capital costs should be a good approximation for the Py-ECH process. A scaling factor of 0.6 was used to account for the change in the amount of feed being handled. The amount of catalyst required was estimated by assuming a weight hourly space velocity (WHSV) of 0.5 hr^{-1}, in accordance with the Dutta et al. report, purchased at $20/lb (in 2011$), with replacement of the initial catalyst every 2 years.[24] Natural gas required for refinery heating was estimated at $ 7.86/1000 cubic feet (in 2007$).[25]

Table S1: Assumptions for Calculating the Total Capital Investment and Total Operating Cost.

Total Installed Capital Cost is the sum of installed equipment costs	
Inside Battery Limits (ISBL) is the total installed capital cost excluding storage	
Direct Costs	
Warehouse	4% of ISBL
Site Development	9% of ISBL
Additional Piping	4.5% of ISBL
Total Direct Cost (TDC) is the sum of all direct costs	
Indirect Costs	
Pro-ratable Costs	10% of TDC
Field Expenses	10% of TDC
Home Office and Construction	10% of TDC
Project Contingency	10% of TDC
Other costs	10% of TDC
Total Indirect Cost (TIC) is the sum of all indirect costs	
Fixed Capital Investment (FCI) is the sum of TDC and TIC	
Land	1.6% of total installed capital cost
Working Capital	5% of FCI
Total Capital Investment (TCI) is the sum of FCI, land, and working capital	
Fixed Operating Cost	
Salaries	0.5% of TCI
Labor Burden	90% of salaries
Maintenance	3% of ISBL
Property Insurance	0.7% of FCI
Total fixed operating cost is the sum of all fixed operating costs	
Total variable operating cost is the sum of variable costs, e.g. utilities and raw materials	
Total Operating Cost is the sum of total fixed and variable operating costs	

Table S2: Range of values of biochar found in literature (adapted from Campbell et al.)[26]

Biochar Price (in 2018$) ($/tonne)	Price Based on	Technology	Description	Citation
230.31	Breakeven price	Pyrolysis	When biochar quantity is maximized @ 300ºC Produced alongside methanol	27
293.12	Breakeven price	Pyrolysis	When biochar quality is maximized @ 450ºC Produced alongside methanol	27

117.44	Energy value	Pyrolysis	Relative to cost of Central Appalachian coal	28
68.34	Soil enhancement ability	Pyrolysis	Includes fertilizer application cost of $40/tonne Includes hauling cost of $8/tonne	29
78.26	Energy value	Fast pyrolysis	Price for optimal temp of 525ºC Yield: bio-oil: 55% and biochar: 20% Max revenue: $118.48/tonne Assumption: Price/unit energy of bio-oil is equal to that of fossil oil Price/unit energy of biochar is equal to that of coal $75/tonne for pyrolysis at 500ºC	30
142.98	Technoeconomic analysis	Pyrolysis	For Sub-Saharan Africa region (Range 99-165) Discount Rate of 10%	31
224.21	Technoeconomic analysis	Pyrolysis	For Northwestern Europe (Range 155-259) Discount Rate of 10%	31
2,868.42	Survey of biochar sellers		US average from survey of 23 companies Based on the survey of 43 companies worldwide, 23 in the US Does not include shipping or handling costs Mix of retail and wholesale prices Mix of pure biochar and blends	32
1,834.00	Communication with industry		Wholesale price	26
88.98	Energy value	Slow pyrolysis	Bio-oil produced (38%) sold at $ 192/tonne Biochar produced (26%) Revenue of $ 93/tonne of forest-based feedstock	33
2,382.94	Market value		Market value for soil amendment @$2.2/kg; possibly retail price	34
414.97	Technoeconomic analysis	Pyrolysis	This is average price in UK Min: $222/tonne; Max: $584/tonne Includes shipping and handling	35
1,763.81	Market survey		Most often cited price Dependent on volume and packaging	36

Table S3: Summary of factors determining assumed costs for corn stover transport to depots as assumed by Kim et al. [37]

$$d_f = w\sqrt{\frac{f_s.h_r/24}{Y_{stover}.r\%.f_{corn}.\pi.f_a.(1-f_l)}}$$

Symbol	Unit	Meaning
$\mathbf{d_f}$	10^2 m	Farm to Depot Distance
$\mathbf{f_s}$	tonnes/day	Facility Size
$\mathbf{h_r}$	hours	Annual operating hours
$\mathbf{f_a}$		Percentage of participating farms
w		Road winding factor
$\mathbf{f_l}$		Transportation and Storage loss factor
$\mathbf{f_{corn}}$		Ratio of harvested corn area to total land

		area
Y_{stover}	tonnes/ha	Dry corn stover yield
r%	%	Fraction of corn stover collected

Table S4: Summary of supply chain costs for corn stover for CE and Py-ECH systems, as used in model.[38] All values in 2018$/tonne of delivered biomass

Supply Chain Operation	CE system ($/tonne)	Py-ECH system ($/tonne)
Harvest and Collection	16.64	16.64
Storage and Handling	3.10	3.10
Grower Payment	38.59	38.59
Transportation and Handling	10.00	2.97
TOTAL	**68.33**	**61.30**

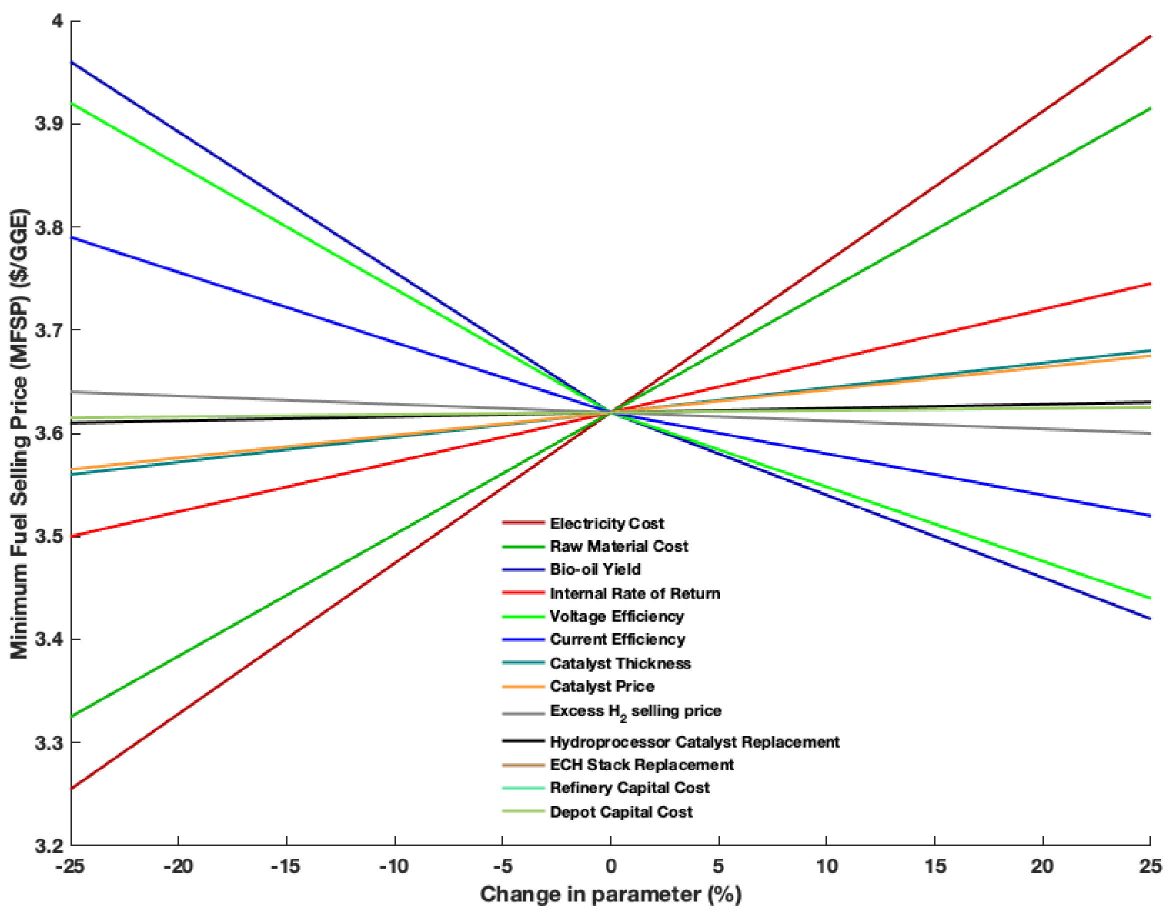

Figure S1: Sensitivity analyses on MFSP for all parameters. The larger the line's slope, the greater the MFSP's sensitivity to that parameter.

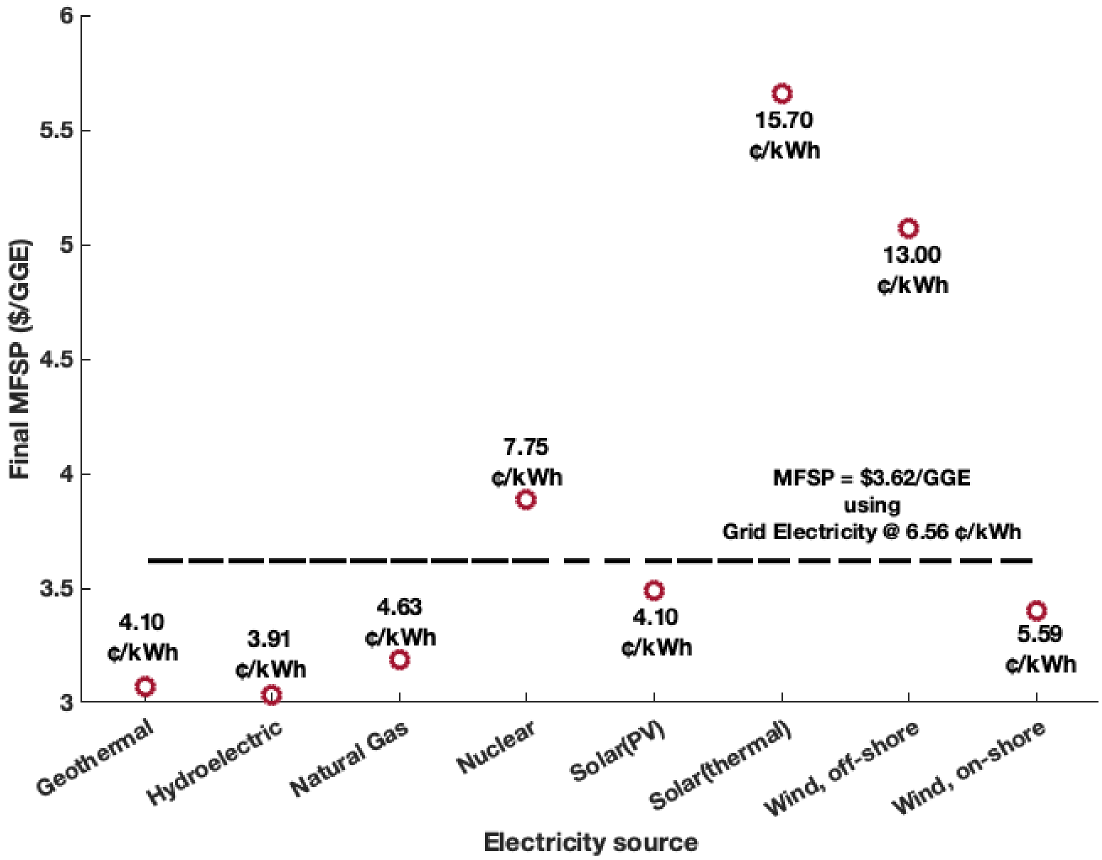

Figure S2: Electricity costs from different sources. Red dashed line indicates the MFSP using MRO-West U.S. grid electricity, assumed as a baseline in the model.[39]

2. Supply Chain Optimization Process

As discussed in the main article, different square depot configurations were assumed, as depicted in Figure 2(a) in the main article. For each configuration, a depot size was assumed, and the average farm-to-depot distance calculated from the geometry. The total number of depots were determined from the central refinery capacity and the assumed depot size. The depots and their collection squares were then randomly placed around the refinery such that there is no overlap between the collection squares of any two depots. It was also assumed that all the depots are located in a square region around the refinery, only 25% of which is dedicated for corn cultivation.[40] No depots were located in the region adjacent to the refinery, denoted by the blue boundary in Figure 2(a), to avoid a situation where the biomass is closer to the refinery than the depot. Any biomass in this region could be directly transported to the refinery where it can be combusted for required heat and power, offsetting natural gas used in the refinery, but increasing the demand for more biomass. This offset was not considered in the present analysis; all heat requirement at the refinery is derived from burning natural gas. Based on the placement of the depots around the refinery, an average depot-to-refinery distance was evaluated. This distance was then minimized over successive iterations, each of which considered a different random arrangement of depots. The arrangement that resulted in the minimum depot-to refinery distance was chosen as the optimal arrangement of depots for that particular depot size. It must also be noted that a circuity factor of 1.23 was assumed for transportation by trucks, as suggested from literature for truck transportation over distances less than 400 km.[37, 41-43]

3. Data Inventory

Table S5: Key ECH and Pyrolysis parameters

Parameter	Value	Source
ECH		
Platinum current density	1,000 mA/cm^2	Kreuter et al.[44]
Platinum thickness	100 nm	
Platinum density	21.45 g/cm^3	
Platinum price	29.33 $/gram	
Nafion 117 conductivity	10 S/m	Liu et al.[45]
Nafion 117 price	2,222.22 $\$/m^2$	
Nafion acid capacity	0.9 meq cations/g dry Nafion	
Nafion thickness	0.1778 mm	
Ruthenium current density	10 mA/cm^2	
Ruthenium thickness	100 nm	
Ruthenium density	12.2 g/cm^3	
Ruthenium price	263 $/troy oz	
ECH Current Efficiency	67%	
ECH Voltage Efficiency	75%	
ECH Temperature	80ºC	
ECH Pressure	1 atm	
Pyrolysis		
Pyrolysis Bio-oil Yield	70%	
Pyrolysis Biochar Yield	15%	
Pyrolysis NCG yield	15%	
Pyrolysis Temperature	500ºC	
Pyrolysis Pressure	1 atm	

Table S6: Installation Multipliers

Processing Unit	Installation Multiplier

At Depot	
Drying	1.70
Grinding	1.70
Pyrolysis	1.80
Condensation	2.20
ECH	1.15
Combustion	1.80
Storage	
At Central Refinery	
Hydroprocessing	1.70
Electrolysis	1.15
Storage	1.80

Table S7: CEPCI Plant Indices

Year	Index
1963	102.4
1964	103.3
1965	104.2
1966	107.2
1967	109.7
1968	113.7
1969	119.0
1970	125.7
1971	132.3
1972	137.2
1973	144.1
1974	165.4
1975	182.4
1976	192.1
1977	204.1
1978	218.8
1979	238.7
1980	261.2
1981	197.0
1982	314.0
1983	317.0
1984	322.7
1985	325.3
1986	318.4
1987	323.8
1988	342.5
1989	355.4

1990	357.6
1991	361.3
1992	358.2
1993	359.2
1994	368.1
1995	381.1
1996	381.7
1997	386.5
1998	389.5
1999	390.6
2000	394.1
2001	394.3
2002	395.6
2003	402.0
2004	444.2
2005	468.2
2006	499.6
2007	525.4
2008	575.4
2009	521.9
2010	550.8
2011	585.7
2012	584.6
2013	567.3
2014	576.1
2015	556.8
2016	541.7
2017	567.5
2018	603.1

1. K. D. T. Max S. Peters, Ronald E. West, Equipment Costs-Plant Design and Economics for Chemical Engineers, http://www.mhhe.com/engcs/chemical/peters/data/.
2. K. D. T. Max S. Peters, Ronald E. West, *Plant Design and Economics for Chemical Engineers*, McGraw Hill, 5th Edition edn.
3. J. R. Hess, K. L. Kenney, P. O. Ovard, E. M. Searcy and C. T. Wright, *Commodity-scale production of an infrastructure-compatible bulk solid from herbaceous lignocellulosic biomass*, Idaho National Laboratory, 2009.
4. T. E. Toolbox, Heat Exchanger Heat Transfer Coefficients, https://www.engineeringtoolbox.com/heat-transfer-coefficients-exchangers-d_450.html.

5. H. Xu, H. Sieverding, H. Kwon, D. Clay, C. Stewart, J. M. F. Johnson, Z. Qin, D. L. Karlen and M. Wang, *GCB Bioenergy*, 2019, **11**, 1215-1233.
6. Z. Li, S. Kelkar, C. H. Lam, K. Luczek, J. E. Jackson, D. J. Miller and C. M. Saffron, *Electrochimica Acta*, 2012, **64**, 87-93.
7. W. An, J. K. Hong and P. Pintauro, *Journal of Applied Electrochemistry*, 1998, **28**, 947-954.
8. M. Garedew, D. Young-Farhat, S. Bhatia, P. Hao, J. E. Jackson and C. M. Saffron, *Sustainable energy & fuels*, 2020, DOI: 10.1039/C9SE00912D.
9. C. H. Lam, C. B. Lowe, Z. Li, K. N. Longe, J. T. Rayburn, M. A. Caldwell, C. E. Houdek, J. B. Maguire, C. M. Saffron, D. J. Miller and J. E. Jackson, *Green Chem.*, 2015, **17**, 601-609.
10. M. Garedew, D. Young-Farhat, J. E. Jackson and C. M. Saffron, *ACS Sustainable Chemistry & Engineering*, 2019, **7**, 8375-8386.
11. P. N. Pintauro, M. P. Gil, K. Warner, G. List and W. Neff, *Industrial & Engineering Chemistry Research*, 2005, **44**, 6188-6195.
12. M. J. Orella, Y. Román-Leshkov and F. R. Brushett, *Current Opinion in Chemical Engineering*, 2018, **20**, 159-167.
13. Z. Li, M. Garedew, C. H. Lam, J. E. Jackson, D. J. Miller and C. M. Saffron, *Green Chemistry*, 2012, **14**, 2540.
14. K. H. Joe Genovese, Mark Paster, John Turner, *Current (2009) State-of-the-Art Hydrogen Production Cost Estimate Using Water Electrolysis*, Report NREL/BK-6A1-46676, NREL, 2009.
15. V. Anantharaman and P. N. Pintauro, *Journal of the Electrochemical Society*, 1994, **141**, 2729-2741.
16. W. G. Colella, B. D. James, J. M. Moton, G. Saur and T. Ramsden, *Techno-economic Analysis of PEM Electrolysis for Hydrogen Production*, NREL, Strategic Analysis Inc., Golden, Colorado, 2013.
17. D. Peterson, J. Vickers and D. DeSantis, *Hydrogen Production Cost From PEM Electrolysis - 2019*, 2020.
18. D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof and M. Worley, *Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol: dilute-acid pretreatment and enzymatic hydrolysis of corn stover*, Report NREL/TP-5100-47764, National Renewable Energy Laboratory (NREL), Golden, CO., 2011.
19. W. A. Amos, *Costs of Storing and Transporting Hydrogen*, Report NREL/TP-570-25106; ON: DE00006574; Other: ON: DE00006574; TRN: US200305%%988 United States 10.2172/6574 Other: ON: DE00006574; TRN: US200305%%988 NREL English, ; National Renewable Energy Lab., Golden, CO (US), 1999.
20. J. R. Keiser, M. Howell, S. A. Lewis and R. M. Connatser, CORROSION 2012.
21. Q. Lu, J. Zhang and X. Zhu, *Chinese Science Bulletin*, 2008, **53**, 3726-3734.
22. J. L. H.P. Loh, Charles W. White, III, *Process Equipment Cost Estimation Final Report*, 2002.
23. S. M. Saba, M. Müller, M. Robinius and D. Stolten, *International Journal of Hydrogen Energy*, 2018, **43**, 1209-1223.

24. A. S. Abhijit Dutta, Eric Tan, David Humbird, Lesley J. Snowden-Swan, Pimphan Meyer, Jeff Ross, Danielle Sexton, Raymond Yap, John Lukas, *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels*, Report NREL/TP-5100-62455 ; PNNL-23823, NREL, PNNL, 2015.
25. *Journal*.
26. R. M. Campbell, N. M. Anderson, D. E. Daugaard and H. T. Naughton, *Energies*, 2018, **11**, 293.
27. S. Shabangu, D. Woolf, E. M. Fisher, L. T. Angenent and J. Lehmann, *Fuel*, 2014, **117**, 742-748.
28. S. P. Galinato, J. K. Yoder and D. Granatstein, *Energy Policy*, 2011, **39**, 6344-6350.
29. C.-C. Kung, B. A. McCarl and X. Cao, *Energy Policy*, 2013, **60**, 317-323.
30. J. Yoder, S. Galinato, D. Granatstein and M. Garcia-Pérez, *Biomass and Bioenergy*, 2011, **35**, 1851-1862.
31. D. Dickinson, L. Balduccio, J. Buysse, F. Ronsse, G. van Huylenbroeck and W. Prins, *GCB Bioenergy*, 2015, **7**, 850-864.
32. S. Jirka and T. Tomlinson, *2013 State of the Biochar Industry: A Survey of Commercial Activity in the Biochar Field*, 2014.
33. C. Granatstein, C. Kruger, H. Collins, S. Galinato, M. Garcia-perez and J. Yoder, *Use of biochar from the pyrolysis of waste organic material as a soil amendment*, 2009.
34. D. Kim, N. M. Anderson and W. Chung, *Forest Products Journal*, 2015, **65**, 189-197.
35. S. Shackley, J. Hammond, J. Gaunt and R. Ibarrola, *Carbon Management*, 2011, **2**, 335-356.
36. K. Draper, H. Groot, T. Miles and M. Twer, *Survey and Analysis of the US Biochar Industry: Preliminary Report Draft (August 16, 2018)*, 2018.
37. S. Kim and B. E. Dale, *Biomass and Bioenergy*, 2015, **74**, 135-147.
38. U. S. D. o. Energy, *Biomass Multi-Year Program Plan*, U.S. Department of Energy, 2011.
39. U. S. E. I. Administration, *Levelized Cost and Levelized Avoided Cost of New Generation Resources in the Annual Energy Outlook 2019*, 2019.
40. S. Sokhansanj, S. Mani, A. Turhollow, A. Kumar, D. Bransby, L. Lynd and M. Laser, *Biofuels, Bioproducts and Biorefining*, 2009, **3**, 124-141.
41. M. Kocoloski, W. Michael Griffin and H. Scott Matthews, *Energy Policy*, 2011, **39**, 47-56.
42. J. L. Thompson and W. E. Tyner, *Biomass and Bioenergy*, 2014, **62**, 166-173.
43. H. L. Wakeley, C. T. Hendrickson, W. M. Griffin and H. S. Matthews, *Environmental Science & Technology*, 2009, **43**, 2228-2233.
44. W. Kreuter and H. Hofmann, *International Journal of Hydrogen Energy*, 1998, **23**, 661-666.
45. L. Liu, W. Chen and Y. Li, *Journal of Membrane Science*, 2016, **504**, 1-9.