1   Energy Utilization Strategies in Lignocellulosic Biorefineries

2   Emmanuel A. Aboagye[1], Christos T. Maravelias[1,2]

3   [1]Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, USA

4   [2]Andlinger Center for Energy and the Environment, Princeton University, Princeton, NJ, USA

5   *Corresponding author: maravelias@princeton.edu

6   Contents

Supplementary Note 1

To estimate the unit production cost parameter, the block capital cost is annualized and divided by the annual processing capacity to determine the unit capital cost (US$ kg^{-1}). This is then combined with the unit operating cost (US$ kg^{-1}) to obtain the total unit production cost.
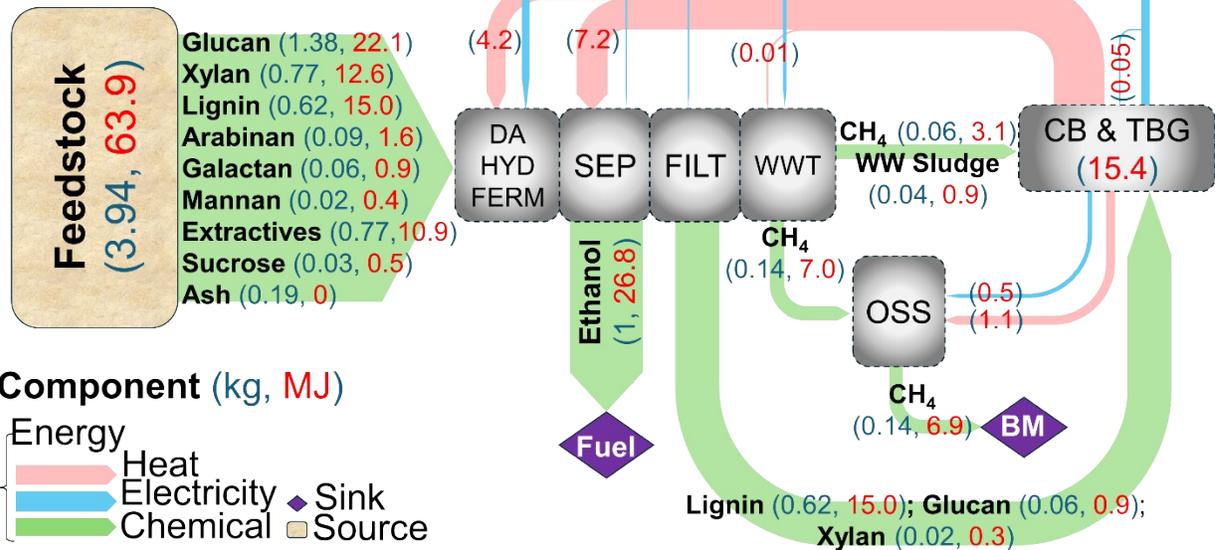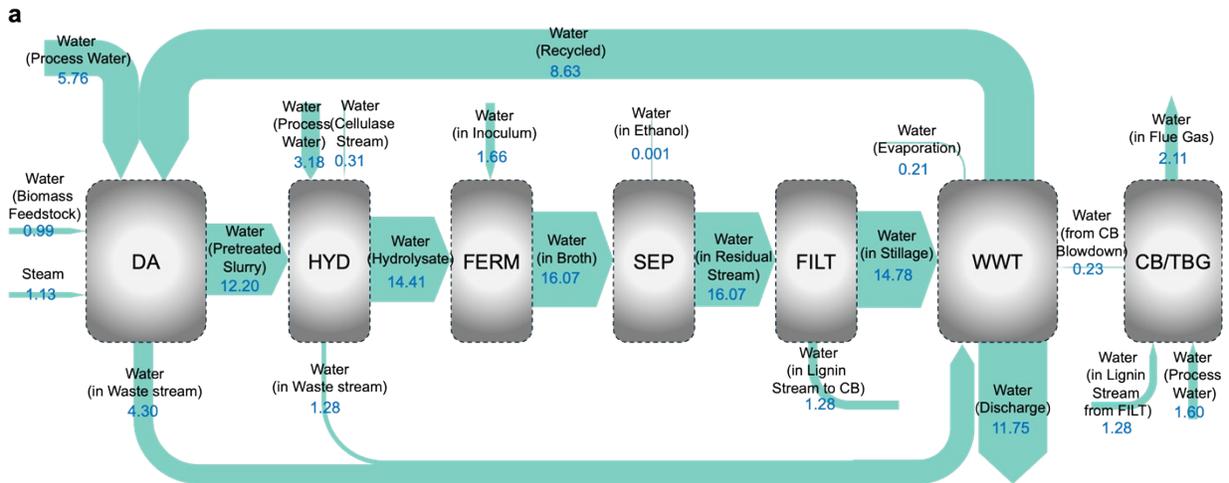
15 **Supplementary Figures**
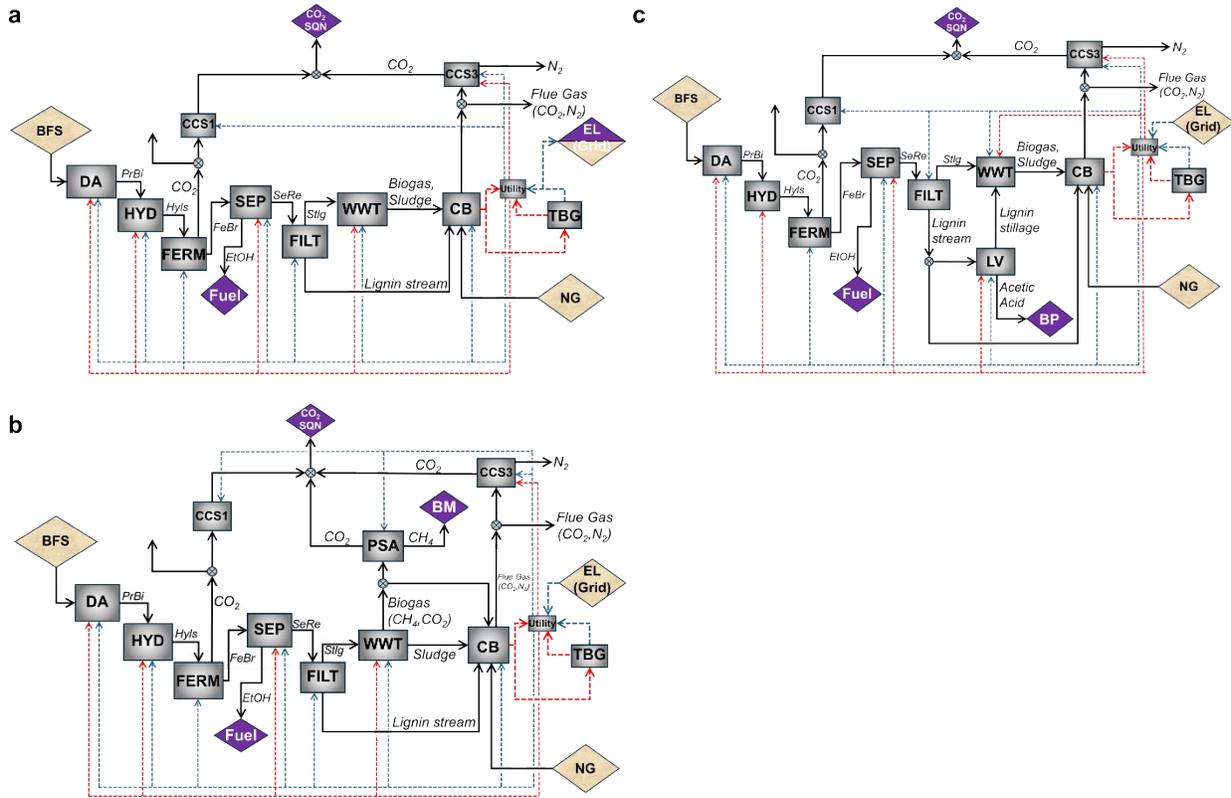
Fig. 1 | Block flow diagram of integrated biorefinery systems (a) $+B_{EL}^{CCS}$. The "El (Grid)" block can act as a source (if we purchase electricity from the grid) or sink (if we sell electricity to the grid) (b) $+B_{BM}^{CCS}$ (c) $+B_{LV}^{CCS}$

3

MFSP: US$4.10 GGE^{-1}
Net CF: 37.3 gCO$_2$e MJ^{-1}

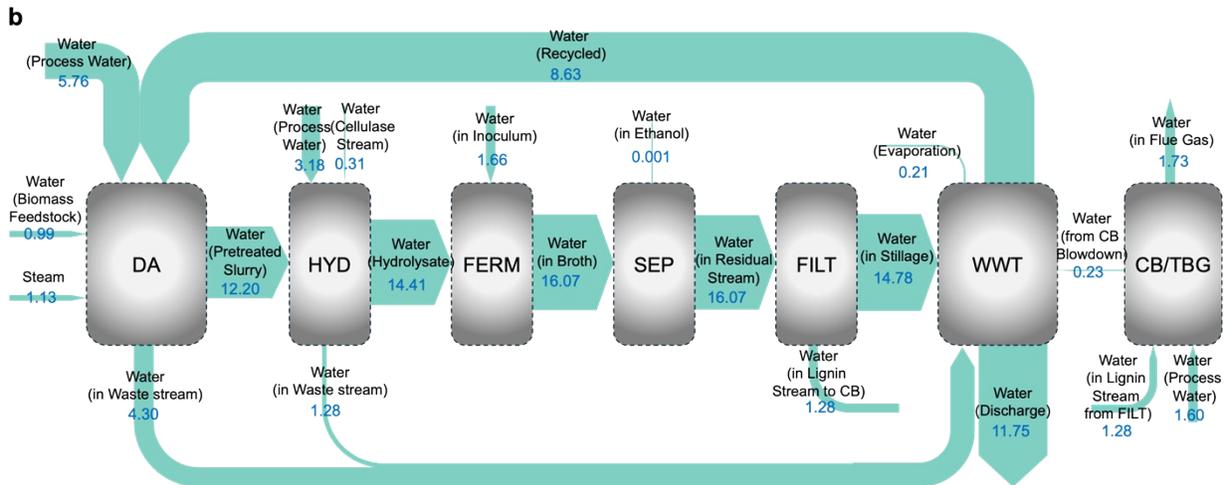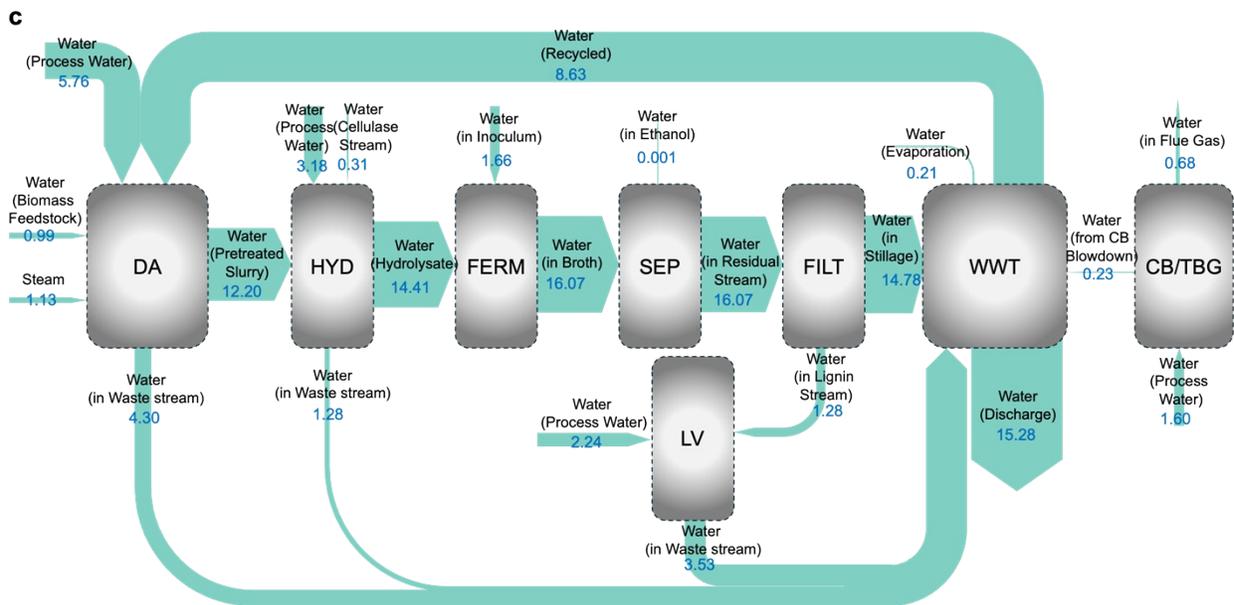Fig. 2 | Energy and mass flow for a B_{BM} system where the upgrading block is changed from pressure swing adsorption (PSA) to organic solvent scrubbing (OSS)[1], which requires both heat and electricity consumption. The heat requirement is primarily due to solvent recovery. The amount of biomethane produced is reduced from 0.16 kg (8.1 MJ) in the baseline where PSA is used to 0.14 kg (7.0 MJ)
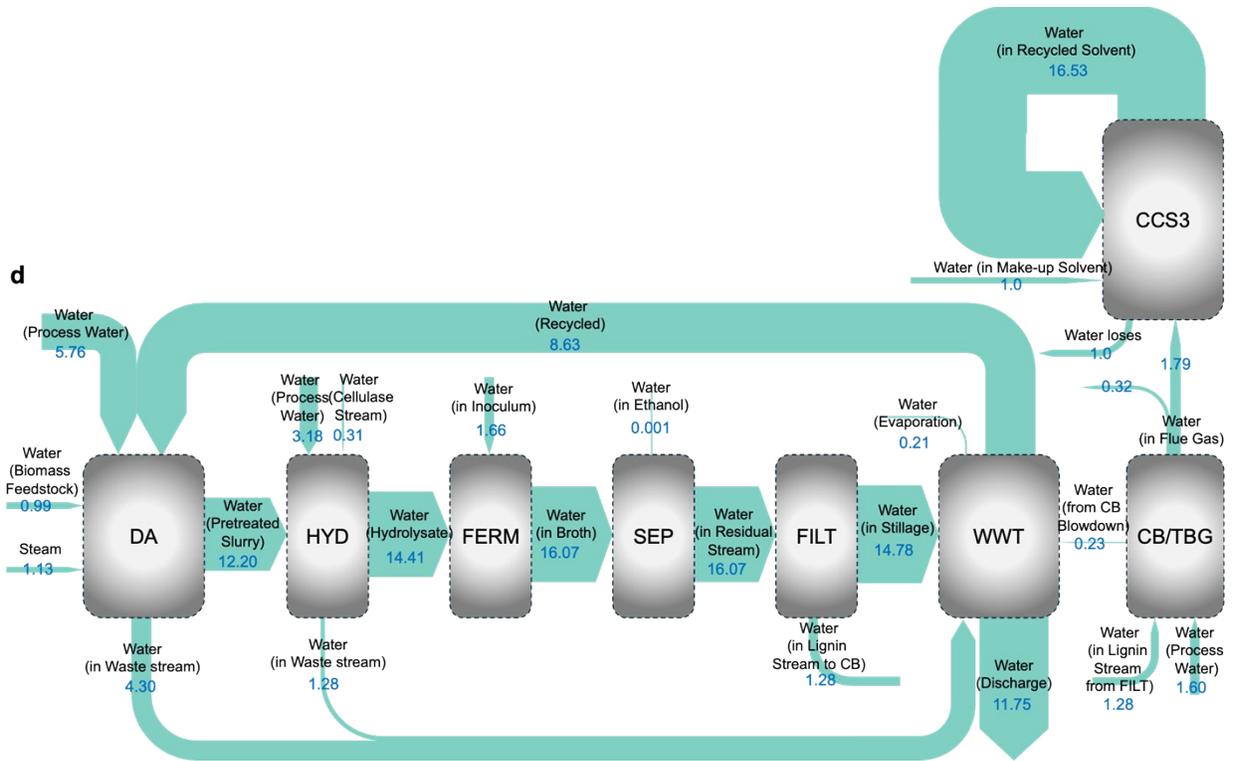
b

Water (Process Water) 5.76

Water (Recycled) 8.63

Water (Process Water) 3.18

Water (Cellulase Stream) 0.31

Water (in Inoculum) 1.66

Water (in Ethanol) 0.001

Water (Evaporation) 0.21

Water (in Flue Gas) 1.73

Water (Biomass Feedstock) 0.99

Steam 1.13

DA

Water (Pretreated Slurry) 12.20

HYD

Water (Hydrolysate) 14.41

FERM

Water (in Broth) 16.07

SEP

Water (in Residual Stream) 16.07

FILT

Water (in Stillage) 14.78

WWT

Water (from CB Blowdown) 0.23

CB/TBG

Water (in Waste stream) 4.30

Water (in Waste stream) 1.28

Water (in Lignin Stream to CB) 1.28

Water (Discharge) 11.75

Water (in Lignin Stream from FILT) 1.28

Water (Process Water) 1.60

26

c

Water (Process Water) 5.76

Water (Recycled) 8.63

Water (Process Water) 3.18

Water (Cellulase Stream) 0.31

Water (in Inoculum) 1.66

Water (in Ethanol) 0.001

Water (Evaporation) 0.21

Water (in Flue Gas) 0.68

Water (Biomass Feedstock) 0.99

Steam 1.13

DA

Water (Pretreated Slurry) 12.20

HYD

Water (Hydrolysate) 14.41

FERM

Water (in Broth) 16.07

SEP

Water (in Residual Stream) 16.07

FILT

Water (in Stillage) 14.78

WWT

Water (from CB Blowdown) 0.23

CB/TBG

Water (in Waste stream) 4.30

Water (in Waste stream) 1.28

Water (Process Water) 2.24

LV

Water (in Lignin Stream) 1.28

Water (Discharge) 15.28

Water (Process Water) 1.60
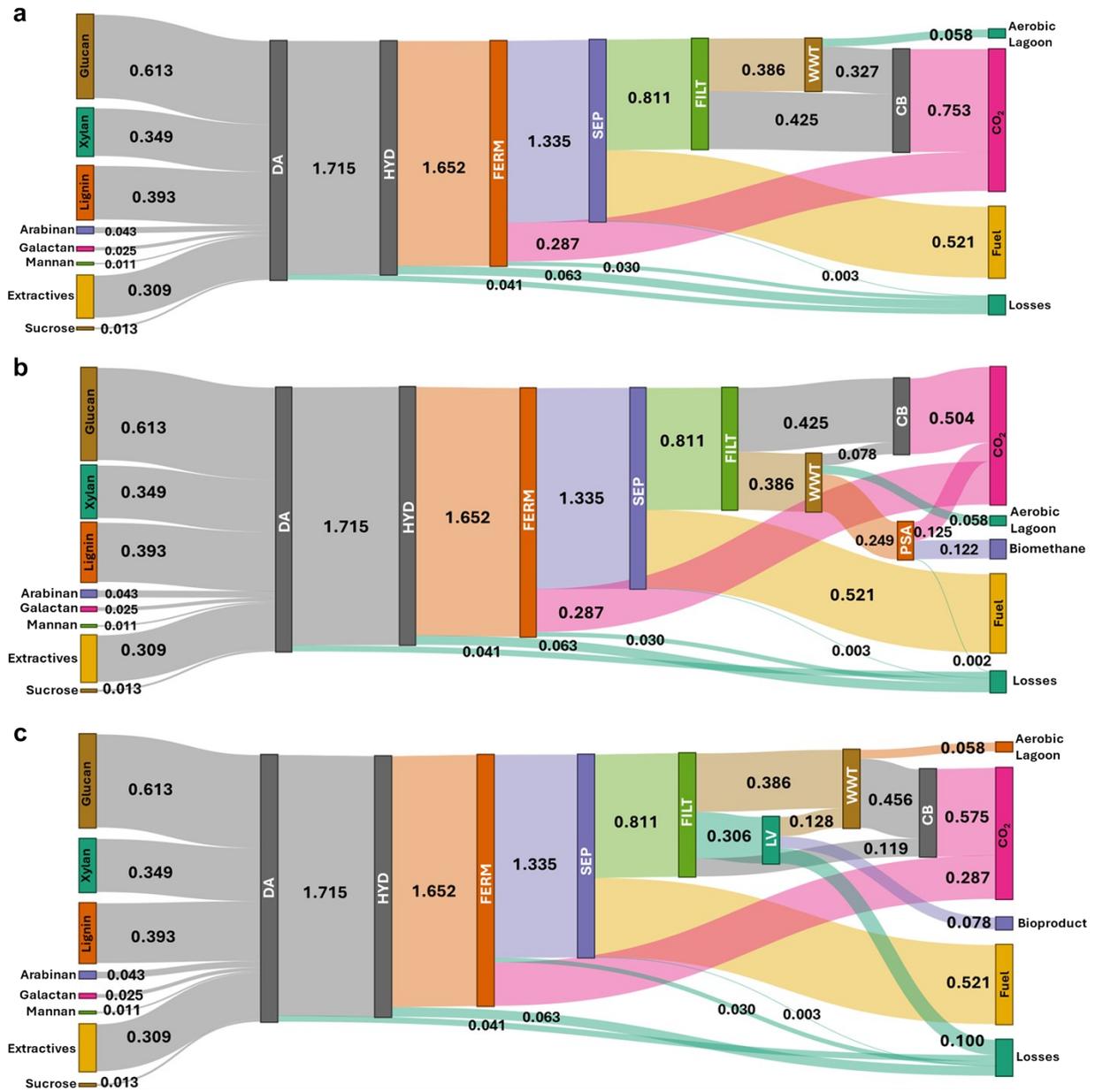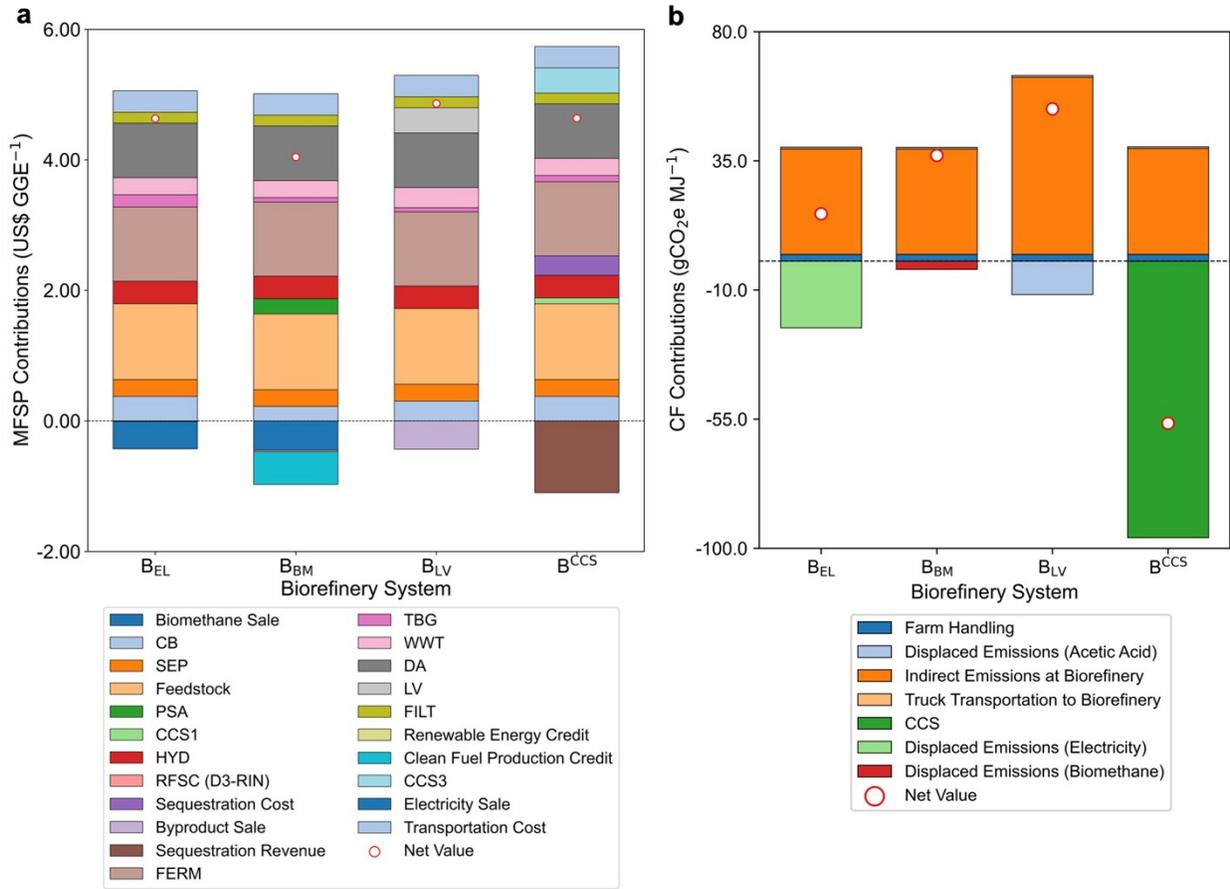
Water (in Waste stream) 3.53

27

5

28

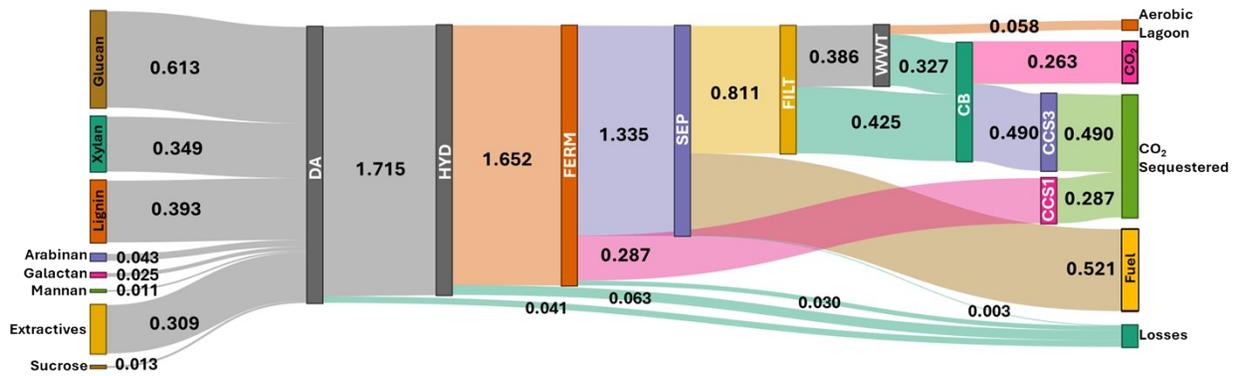29   Fig. 3 | Water flow for 1 kg of fuel produced. (a) B_{EL} (b) B_{BM} (c) B_{LV}(d) B^{CCS}

Fig. 4 | Carbon flow for 1 kg of fuel produced. (a) B_{EL} (b) B_{BM} (c) B_{LV}

32

33 Fig. 5 | MFSP and CF breakdown of each baseline system. (a) MFSP (b) CF

34

35

36 Fig. 6 | Carbon flow for 1 kg of fuel produced for B^{CCS} system

37
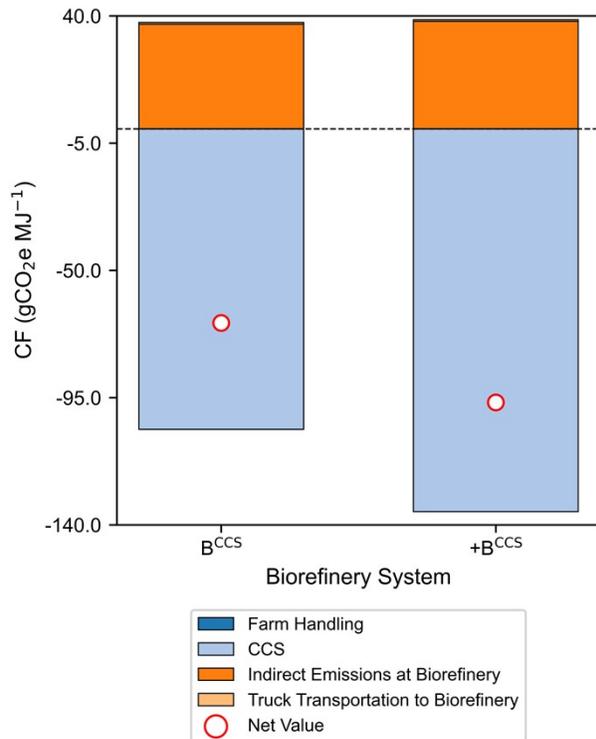
Fig. 7 | Solution for the biorefinery with carbon capture system, with ($+B^{CCS}$) and without (B^{CCS}) natural gas purchase

40
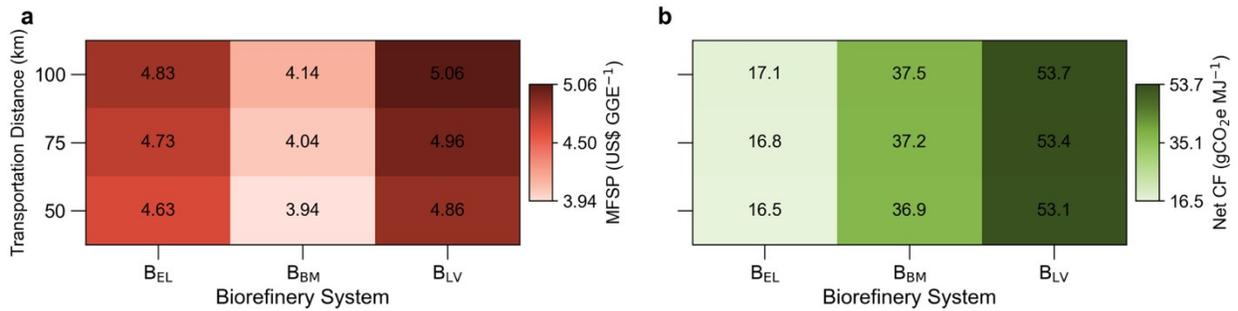
Fig. 8 | Impact of average biomass transportation (truck) distance on (a) MFSP and (b) net CF for the three co-production baseline systems. MFSP increased by ~4-5% across all systems, with no change in relative ranking.

43

44 Supplementary Tables

45 Table 1. Corn Stover composition[2]

Component	Composition (kg kg^{-1})
Xylan	0.195
Glucan	0.350
Lignin	0.158
Arabinan	0.024
Galactan	0.014
Mannan	0.006
Extractives	0.196
Sucrose	0.008
Ash	0.049

46 Table 2. Lower heating value[2] of components

Component	LHV (kWh kg^{-1})
Glucan	4.441
Xylan	4.564
Lignin	6.681
Ash	0.000
Extractives	3.935
Arabinan	4.564
Galactan	4.441
Mannan	4.441
Sucrose	4.354
Ethanol	7.441
Xylose	3.943
Arabinose	3.943
Galactose	3.935
Mannose	3.935
HMF	5.875
Furfural	6.504
WWSludge	5.921
CH_4	13.890
AceticAcid	3.765
CO_2	0.000
Glucose	3.935
NaturalGas	13.890

47 (NB: We modeled extractives, galactose, and mannose after glucose, arabinan after xylan, galactan and mannan after glucan,
48 and arabinose after xylose)

49 Table 3. Conversion coefficients of components in each block[2–5]

i	i'	j	j'	$\eta_{i,i',j,j'}$
Xylan	Furfural	DA	HYD	0.050
Xylan	Xylose	DA	HYD	0.924
Xylan	Xylan	DA	HYD	0.020
Glucan	Glucose	DA	HYD	0.102

10

Glucan	HMF	DA	HYD	0.003
Glucan	Glucan	DA	HYD	0.895
Lignin	Lignin	DA	HYD	1.000
Arabinan	Arabinan	DA	HYD	1.000
Galactan	Galactan	DA	HYD	1.000
Mannan	Mannan	DA	HYD	1.000
Extractives	Extractives	DA	HYD	1.000
Sucrose	Glucose	DA	HYD	1.000
Ash	Ash	DA	HYD	1.000
Xylan	Xylan	HYD	FERM	1.000
Xylose	Xylose	HYD	FERM	1.000
Glucan	Glucose	HYD	FERM	0.954
Glucan	Glucan	HYD	FERM	0.046
Lignin	Lignin	HYD	FERM	1.000
Furfural	Furfural	HYD	FERM	1.000
HMF	HMF	HYD	FERM	1.000
Arabinan	Arabinose	HYD	FERM	0.970
Galactan	Galactose	HYD	FERM	0.970
Mannan	Mannose	HYD	FERM	0.970
Extractives	Extractives	HYD	FERM	1.000
Glucose	Glucose	HYD	FERM	1.000
Ash	Ash	HYD	FERM	1.000
Glucose	CO_2	FERM	SPLT1	0.489
Xylose	CO_2	FERM	SPLT1	0.489
Arabinose	CO_2	FERM	SPLT1	0.489
HMF	HMF	FERM	SEP	1.000
Furfural	Furfural	FERM	SEP	1.000
Ash	Ash	FERM	SEP	1.000
Glucan	Glucan	FERM	SEP	1.000
Glucose	Glucose	FERM	SEP	0.025
Extractives	Extractives	FERM	SEP	0.950
Lignin	Lignin	FERM	SEP	1.000
Xylose	Xylose	FERM	SEP	0.076
Xylose	Ethanol	FERM	SEP	0.435
Glucose	Ethanol	FERM	SEP	0.486
Arabinose	Ethanol	FERM	SEP	0.435
Mannose	Mannose	FERM	SEP	1.000
Galactose	Galactose	FERM	SEP	1.000
Xylan	Xylan	FERM	SEP	1.000
Ethanol	Ethanol	SEP	FUEL	0.995
Xylan	Xylan	SEP	FILT	1.000
Glucan	Glucan	SEP	FILT	1.000
Lignin	Lignin	SEP	FILT	1.000
Glucose	Glucose	SEP	FILT	1.000
Xylose	Xylose	SEP	FILT	1.000
HMF	HMF	SEP	FILT	1.000
Furfural	Furfural	SEP	FILT	1.000
Ash	Ash	SEP	FILT	1.000
Extractives	Extractives	SEP	FILT	1.000
Mannose	Mannose	SEP	FILT	1.000
Galactose	Galactose	SEP	FILT	1.000
Xylan	Xylan	FILT	SPLT2	1.000
Glucan	Glucan	FILT	SPLT2	1.000
Lignin	Lignin	FILT	SPLT2	1.000
Glucose	Glucose	FILT	WWT	1.000

Xylose	Xylose	FILT	WWT	1.000
HMF	HMF	FILT	WWT	1.000
Furfural	Furfural	FILT	WWT	1.000
Ash	Ash	FILT	WWT	1.000
Extractives	Extractives	FILT	WWT	1.000
Mannose	Mannose	FILT	WWT	1.000
Galactose	Galactose	FILT	WWT	1.000
Glucose	CH_4	WWT	SPLT3	0.227
Xylose	CH_4	WWT	SPLT3	0.227
Extractives	CH_4	WWT	SPLT3	0.227
Mannose	CH_4	WWT	SPLT3	0.227
Galactose	CH_4	WWT	SPLT3	0.227
Glucose	CO_2	WWT	SPLT3	0.623
Xylose	CO_2	WWT	SPLT3	0.623
Extractives	CO_2	WWT	SPLT3	0.623
Mannose	CO_2	WWT	SPLT3	0.623
Galactose	CO_2	WWT	SPLT3	0.623
HMF	WWSludge	WWT	CB	0.050
Furfural	WWSludge	WWT	CB	0.050
Ash	Ash	WWT	CB	0.050
Extractives	WWSludge	WWT	CB	0.050
Mannose	WWSludge	WWT	CB	0.050
Galactose	WWSludge	WWT	CB	0.050
Lignin	Lignin	WWT	CB	1.000
Xylan	Xylan	WWT	CB	1.000
Glucan	Glucan	WWT	CB	1.000
Lignin	AceticAcid	LV	BP	0.390
Xylan	AceticAcid	LV	BP	0.390
Glucan	AceticAcid	LV	BP	0.390
Xylan	Xylan	LV	WWT	0.367
Glucan	Glucan	LV	WWT	0.420
Lignin	Lignin	LV	WWT	0.420
CO_2	CO_2	CB	SPLT4	1.000
CH_4	CO_2	CB	SPLT4	2.749
Xylan	CO_2	CB	SPLT4	1.666
Glucan	CO_2	CB	SPLT4	1.629
WWSludge	CO_2	CB	SPLT4	1.894
Lignin	CO_2	CB	SPLT4	2.314
CH_4	N_2	CB	SPLT4	13.63
Xylan	N_2	CB	SPLT4	4.130
Glucan	N_2	CB	SPLT4	4.039
WWSludge	N_2	CB	SPLT4	5.772
Lignin	N_2	CB	SPLT4	6.097
CO_2	CO_2	CCS1	SQN	1.000
CO_2	CO_2	CCS2	SQN	0.980
CH_4	CH_4	CCS2	CB	1.000
CO_2	CO_2	CCS3	SQN	0.850
N_2	N_2	CCS3	VENT	1.000
NaturalGas	CO_2	CB	SPLT4	2.749
NaturalGas	N_2	CB	SPLT4	13.63
CH_4	CH_4	PSA	BM	0.980
CO_2	CO_2	PSA	SPLT5	1.000

Table 4. Unit consumption of auxiliary chemicals by blocks for indirect emission accounting[2-4]

i	j	Unit	$\rho_{i,j}$
H_2SO_4	DA	kg/kg dry biomass	0.0090
NH_3	DA	kg/kg dry biomass	0.0303
Caustic	DA	kg/kg dry biomass	0.0170
CSL	FERM	kg/kg hydrolysate	0.0005
NH_3	FERM	kg/kg hydrolysate	0.0012
Glucose	FERM	kg/kg hydrolysate	0.0014
Caustic	WWT	kg/kg wastewater	0.4850
FGD	CB	kg/kg flue gas	0.0029
Ethanol	LV	kg/kg lignin	0.0054
NH_3	LV	kg/kg lignin	0.3520
CSL	LV	kg/kg lignin	0.0315
H_2SO_4	LV	kg/kg lignin	1.4359

(NB: we assume that the enzyme used for fermentation is produced onsite and it is included in the fermentation block. FGD: Flue gas desulfurization lime, CSL: Corn steep liquor)

Table 5. Additional process and economic related parameters[2,4,6-8]

General parameters	Units	Value
Feedstock purchase price ($\gamma_{i=cornstover}^{PP}$)	$ kg^{-1}	0.06485
Natural gas purchase price ($\gamma_{i=naturalgas}^{PP}$)	$ kg^{-1}	0.6
Electricity price ($\gamma_{i=electricity}^{PP/SP}$)	$ kWh^{-1}	0.0572
Average biomass transportation distance (ϑ)*	km	50
Biomethane (CH_4) selling price ($\gamma_{i=CH4}^{SP}$)	$ kg^{-1}	0.6
Acetic acid selling price ($\gamma_{i=aceticacid}^{SP}$)	$ kg^{-1}	0.5
Renewable Identification Number (D3-RIN) credit ($\pi_{i=CH4}$)**	$ kg^{-1}	0.032 – 2.27
Clean fuel production credit ($\pi_{i=CH4}$)**	$ kg^{-1}	0.68 – 1.14
Renewable energy credits ($\pi_{i=electricity}$)	$ kWh^{-1}	0.001
Fixed cost for biomass truck transportation (τ^{TF})	$ kg^{-1}	0.0075
Variable cost for biomass truck transportation (τ^{TV})	$ kg^{-1} km^{-1}	0.000218
Sequestration cost (τ^{SQN})	$ kg^{-1}	0.02
Biofuel demand (β)	kg	1
Gasoline gallon equivalent per kg of ethanol (ζ)	GGE kg^{-1}	0.22
Truck transportation emission factor (ξ^{TR})	kgCO$_2$e kg^{-1} km^{-1}	0.000080
Farm handling emission factor (ξ^{FH})	kgCO$_2$e kg^{-1}	0.016

*Assumed value, **Converted to per kg of biomethane

Table 6. Unit production cost, electricity, and heat demand for each block[1-4,9]

j	Production cost, μ_j ($ kg^{-1} or $ kWh^{-1}*)	Electricity, $\delta_{i=electricity,j}$ (kWh kg^{-1})	Heat, $\delta_{i=heat,j}$ (kWh kg^{-1})
DA	0.047	0.096	0.204
HYD	0.019	0.016	0.094
FERM	0.064	0.016	-

SEP	0.020	0.013	0.707
FILT	0.020	0.013	-
WWT	0.051	0.088	0.003
CB	0.054	0.016	-
LV	0.170	0.127	0.833
CCS1	0.019	0.151	-
CCS2	0.086	0.230	-
CCS3	0.047	0.175	0.793
TBG	0.007*	-	-
PSA	0.086	0.230	-

56

57 Table 7. 5-year average electricity price, grid emission factor, and biomethane price for each state
58 in the US between 2019 - 2023[10,11]

State id	State Name	Price ($ kWh^{-1}), $\gamma_{i=electricity}^{SP}$	*Price($ kg^{-1}), $\gamma_{i=CH4}^{SP}$	Emission Factor (kg CO$_2$e kWh^{-1}), $\xi_{i=electricity}$
AL	Alabama	0.1058	0.8414	0.3417
AZ	Arizona	0.1104	0.7869	0.3446
AR	Arkansas	0.0906	0.7012	0.4747
CA	California	0.2035	0.8475	0.1978
CO	Colorado	0.1097	0.4831	0.5478
CT	Connecticut	0.2029	0.8193	0.2349
DE	Delaware	0.1119	0.7031	0.3573
DC	District of Columbia	0.1368	0.7191	0.2904
FL	Florida	0.1144	1.1651	0.3795
GA	Georgia	0.1066	0.8266	0.3468
ID	Idaho	0.0833	0.3765	0.1142
IL	Illinois	0.1063	0.5144	0.2727
IN	Indiana	0.1067	0.5015	0.7138
IA	Iowa	0.0923	0.5057	0.3181
KS	Kansas	0.1068	0.5816	0.3721
KY	Kentucky	0.0936	0.6376	0.7878
LA	Louisiana	0.0867	0.6808	0.3654
ME	Maine	0.1596	0.8660	0.1280
MD	Maryland	0.1231	0.7404	0.2947
MA	Massachusetts	0.2003	0.8664	0.3804
MI	Michigan	0.1272	0.4794	0.4327
MN	Minnesota	0.1125	0.4917	0.3637
MS	Mississippi	0.0984	0.6440	0.3887
MO	Missouri	0.1006	0.6262	0.7108
MT	Montana	0.0972	0.4341	0.4830
NE	Nebraska	0.0897	0.5105	0.5199
NV	Nevada	0.0994	0.5879	0.3170
NH	New Hampshire	0.1904	0.8754	0.1265
NJ	New Jersey	0.1423	0.5520	0.2248
NM	New Mexico	0.0952	0.4700	0.4982
NY	New York	0.1639	0.7185	0.2017
NC	North Carolina	0.0968	0.7416	0.3070
ND	North Dakota	0.0850	0.4324	0.6174
OH	Ohio	0.1009	0.5647	0.5390
OK	Oklahoma	0.0867	0.5815	0.3209
OR	Oregon	0.0923	0.6075	0.1570

PA	Pennsylvania	0.1078	0.6503	0.3217
RI	Rhode Island	0.1928	0.8461	0.3779
SC	South Carolina	0.1022	0.7339	0.2485
SD	South Dakota	0.1028	0.4518	0.1633
TN	Tennessee	0.1011	0.5243	0.3023
TX	Texas	0.0926	0.6934	0.3836
UT	Utah	0.0854	0.4850	0.6971
VT	Vermont	0.1651	0.7242	0.0201
VA	Virginia	0.0985	0.7175	0.2727
WA	Washington	0.0875	0.6031	0.1059
WV	West Virginia	0.0922	0.5770	0.8865
WI	Wisconsin	0.1143	0.4680	0.5483
WY	Wyoming	0.0825	0.5363	0.8670

59 *NB: we assume natural gas prices as selling price of biomethane. This assumption is conservative as biomethane (RNG)
60 prices tend to even be higher than natural gas. For the emission factor, we use the average national emission factor.

61 Table 8. Component emission factors[12]

i	ξ_i (kgCO$_2$e kg^{-1}, kgCO$_2$e kWh^{-1}*)
NaturalGas	0.463
Electricity (average US Grid)	0.386*
Electricity (coal power plant)	1.195*
Electricity (natural gas power plant)	0.683*
Electricity (nuclear power plant)	0.009*
Electricity (diesel power plant)	1.164*
Caustic	1.105
NH$_3$	2.265
Glucose	1.516
H$_2$SO$_4$	0.145
CSL	2.992
Ethanol	2.136
FGD	1.104
AceticAcid	1.633

Supplementary Methods

Main Sets

$i \in I$ components

$j \in J$ blocks

Subsets

$I^F \subset I$ biomass feedstocks

$I^R \subset I$ resource (natural gas and electricity)

$I^I \subset I$ intermediates

$I^E \subset I$ energy (heat and electricity)

$I^B \subset I$ biofuel

$I^S \subset I$ sink components

$I^G \subset I$ auxiliary components

$J^{DA} \subset J$ pretreatment

$J^{CMB} \subset J$ combustion

$J^{TBG} \subset J$ turbogenerator

$J^{SNK} \subset J$ sinks

$J^{SPL} \subset J$ splitters

$J^{CF} \subset J$ blocks requiring auxiliary components

$J^{CSPL}_{(j,j')} \subset J$ splitter j connected to downstream block j'

Parameters

β biofuel demand (kg)

ε emission constraint value (kg CO_2e kWh^{-1})

$\alpha_{i,i'}$ fraction of component i in feedstock i' (feed composition, kg kg^{-1})

$\delta_{i,j}$ energy demand i (heat and electricity) of block j (kWh kg^{-1})

$\eta_{i,i',j,j'}$ conversion of component i to component i' in block j which flows into block j' (--)

μ_j production cost of block j (US\$ kg^{-1} or US\$ kWh^{-1})

κ_i heat of combustion (Lower Heating Value) of component i (kWh kg^{-1})

ω^{CB}/ω^{TBG} efficiency of CB (chemical-to-heat) and TBG (heat-to-power) blocks (--)

φ^{TBG} heat recovery in TBG block (--)

$\gamma^{SP}_i/\gamma^{PP}_i$ selling/purchase price of component (US\$ kg^{-1} or US\$ kWh^{-1})

π_i financial incentive for co-product, i (US\$ kg^{-1} or US\$ kWh^{-1})

$\rho_{i,j}$ requirement of auxiliary component i by block, j (for indirect emissions) (kg kg^{-1})

ξ^{FH}/ξ^{TR} biomass farm handling/transportation emission factor (kgCO_2e kg^{-1}/kgCO_2e kg^{-1} km^{-1})

ξ_i emission factor of auxiliary and resource component i (kgCO_2e kg^{-1} or kgCO_2e kWh^{-1})

σ^M upper bound on block consumption, and electricity and natural gas purchase

ϑ average biomass feedstock transportation distance (km)

$\tau^{TF}/\tau^{TV}/\tau^{SQN}$ fixed/variable biomass transportation cost/sequestration cost (US\$ kg^{-1}/ US\$ kg^{-1} km^{-1}/US\$ kg^{-1})

104	ζ	gasoline gallon equivalent per kg of ethanol (GGE kg^{-1})
105		
106		

107 Variables

108	F^{SR}_i / F^{SK}_i	mass flow of component i from/toward source/sink (kg)
109	$F^{IN}_{i,j} / F^{OUT}_{i,j}$	mass flow of component i into/out of block j (kg)
110	$F_{i,j,j'}$	mass flow of component i from block j to j' (dummy flow between blocks, kg)
111	$S_{j,j'}$	fraction of flow split between splitter block j and downstream block j' (--)
112	E^{UT}_i	total energy requirement i (heat and electricity) of biorefinery (kWh)
113	E^{SR}_i / E^{SK}_i	energy flow of component i (heat and electricity) from/toward source/sink (kWh)
114	$E^{IN}_{i,j} / E^{OUT}_{i,j}$	energy flow of component i (heat and electricity) into/out of block, j (kg)
115	$Z^E/Z^N/Y_j$	=1 if electricity/natural gas is purchase/block j is selected (binary variables)
116	C	total cost ($)
117	$C^{FES}/C^{TRN}/C^{PRD}/C^{UTL}/C^{SQN}$	
118		feedstock/transportation/production/utility/sequestration costs ($)
119	R^{COP}/R^{CCS}	co-product/carbon capture and storage revenue ($)
120	G	net carbon footprint (kg CO$_2$e)
121	$G^{BRN}/G^{DIP}/G^{CCS}$	
122		farm handling, transportation, material and energy inputs footprint/avoided
123		emission footprint/captured carbon (kg CO$_2$e)
124		

125 Equations

126 *Material Balance*

127 Feedstock flow from source to pretreatment block is given by:

$$\sum_{i' \in I^F} \alpha_{i',i} F^{SR}_{i'} = \sum_{j \in J^{DA}} F^{IN}_{i,j} \quad ; \forall\, i \in I^I \#(1)$$

128

129 Flow of component into and out of blocks is given by:

$$F^{IN}_{i,j} = \sum_{j'} F_{i,j',j} \quad ; \forall\, i \in I^I, j \in J\backslash(J^{DA} \cup J^{TBG}) \#(2)$$

130

$$F^{OUT}_{i',j} = \sum_{j'} F_{i',j,j'} ; \forall\, i' \in I^I, j \in J\backslash J^{SNK} \#(3)$$

131

132 The conversion (mass) of component in blocks is given by:

$$F_{i',j,j'} = \sum_{i \in I^I} \eta_{i,i',j,j'} F^{IN}_{i,j} \quad ; \forall\, i' \in I^I, j \in J\backslash J^{SPL}, j' \in J \#(4)$$

133

134 The flow from the outlet of some blocks can be split, and that is given by:

135 $$F_{i',j,j'} = S_{j,j'} F^{OUT}_{i',j} \quad ; \forall\, i' \in I^I, (j,j') \in J^{CSPL}_{(j,j')} \#(5)$$

136 The summation of the split fraction between splitter and corresponding connected downstream
137 blocks should be unity for all splitter blocks. That is given by:

138 $$\sum_{\substack{J^{CSPL} \\ (j,j')}} S_{j,j'} = 1 \ ; \forall \ j \in J^{SPL} \ \#(6)$$

139 Natural gas requirement is given by:

140 $$F_i^{SR} = \sum_{j \in J^{CMB}} F_{i,j}^{IN} \ ; \forall \ i \in I^R \backslash I^E \#(7)$$

141 Flow of components to sinks is given by:

142 $$F_i^{SK} = \sum_{j' \in J, j \in J^{SNK}} F_{i,j',j} \ ; \forall \ i \in I^S \#(8)$$

143 ***Energy Balance***

144 The total biorefinery energy (heat and electricity) demand is given by:

145 $$E_i^{UT} = \sum_{j \in J} \delta_{i,j} X_j \ ; \forall \ i \in I^E \ \#(9)$$

146 The total heat generated by combustor block is given by:

147 $$E_{i = heat,j}^{OUT} = \sum_{i \in I^I \cup I^R \backslash I^E} \omega^{CB} \kappa_i F_{i,j}^{IN} \ ; \forall \ j \in J^{CMB} \#(10)$$

148 The heat balance for the biorefinery is given:

149 $$E_{i = heat}^{UT} = \sum_{j \in J^{CMB}} E_{i = heat,j}^{OUT} - \sum_{j \in J^{TBG}} \left(1 - \varphi^{TBG}\right) E_{i = heat,j}^{IN} \#(11)$$

150 The electricity generated by the turbogenerator is given by:

151 $$E_{i = electricity,j}^{OUT} = \omega^{TBG} E_{i = heat,j}^{IN} \ ; \forall \ j \in J^{TBG} \#(12)$$

152 The electricity balance for the biorefinery is given:

153 $$E_{i = electricity}^{UT} + E_{i = electricity}^{SK} = \sum_{j \in J^{TBG}} E_{i = electricity,j}^{OUT} + E_{i = electricity}^{SR} \#(13)$$

154 ***Bounds, demand and block consumption***

155 Consumption level in blocks is given by:

156 $$X_j = \sum_{i \in I^I \cup I^R \backslash I^E} F_{i,j}^{IN} \ ; \forall \ j \in J \backslash J^{TBG} \ \#(14)$$

157 $$X_j = \sum_{i \in I^E} E_{i,j}^{IN} \ ; \forall \ j \in J^{TBG} \ \#(15)$$

158 $$X_j \leq \sigma^M \ Y_j \ \forall \ j \in J \#(16)$$

159 Logical equation for if electricity is purchased or sold (if we purchase electricity from the grid, then

160 we cannot sell electricity to the grid):

161 $$E_{i = electricity}^{SR} \leq \sigma^M Z^E \#(17)$$

162 $$E_{i = electricity}^{SK} \leq \sigma^M (1 - Z^E) \#(18)$$

163 Logical equation for natural gas purchase:

164 $$F_i^{SR} \leq \sigma^M Z^N \ ; \forall \ i \in I^R \backslash I^E \#(19)$$

165 Biofuel demand:

166 $$F_{i = ethanol}^{SK} = \beta \ \#(20)$$

167 *Economics*

168 The objective function, which is total cost is given by (same as Equation (1) in main text):

169 $$C = C^{FES} + C^{TRN} + C^{PRD} + C^{UTL} + C^{SEQ} - (R^{COP} + R^{CCS}) \#(21)$$

170 The following equations give the expression for the cost terms.

171 The biomass feedstock purchase cost is given by:

172 $$C^{FES} = \sum_{i \in I^F} \gamma_i^{PP} F_i^{SR} \#(21a)$$

173 The transportation cost, which has a fixed and variable term, is given by:

174 $$C^{TRN} = \sum_{i \in I^F} (\tau^{TF} + \tau^{TV} \vartheta) F_i^{SR} \#(21b)$$

175 The production cost is given by:

176 $$C^{PRD} = \sum_{j \in J} \mu_j X_j \#(21c)$$

177 The utility cost comprising natural gas and electricity is given by:

178 $$C^{UTL} = \sum_{i \in I^R \backslash I^E} \gamma_i^{PP} F_i^{SR} + \sum_{i \in I^R \cap I^E} \gamma_i^{PP} E_i^{SR} \#(21d)$$

179 The sequestration cost is given by:

180 $$C^{SEQ} = \tau^{SQN} F_{i=CO2}^{SK} \#(21e)$$

181 The total revenue from co-products and carbon capture is given by:

182 $$(R^{COP} + R^{CCS}) = \sum_{i \in I^S \backslash (I^E \cup I^B)} (\pi_i + \gamma_i^{SP}) F_i^{SK} + \sum_{i \in I^S \cap I^E} (\pi_i + \gamma_i^{SP}) E_i^{SK} \#(21f)$$

183 *Carbon Footprint*

184 The net carbon footprint is given by (same as Equation (2) in main text):

185 $$G = G^{BRN} - (G^{DIP} + G^{CCS}) \#(22)$$

186 Carbon footprint due to farm handling and transportation of feedstock, natural gas and
187 electricity requirements, additional component requirements is given by:

188 $$G^{BRN} = \sum_{i \in I^F} (\xi^{FH} + \xi^{TR} \vartheta) F_i^{SR} + \sum_{i \in I^R \backslash I^E} \xi_i F_i^{SR} + \sum_{i \in I^R \cap I^E} \xi_i E_i^{SR} + \sum_{i \in I^G, j \in J^{CF}} \rho_{i,j} \xi_i X_j \#(22a)$$

189 Avoided emission and captured carbon is given by:

190 $$(G^{DIP} + G^{CCS}) = \sum_{i \in I^S \backslash (I^E \cup I^B)} \xi_i F_i^{SK} + \sum_{i \in I^S \cap I^E} \xi_i E_i^{SK} \#(22b)$$

191

192 We determine the minimum fuel selling price (MFSP) on a gasoline gallon equivalent (US\$ GGE^{-1}) and
193 the net carbon footprint (CF) on a gram carbon dioxide equivalent per megajoule of ethanol (g CO_2e
194 MJ^{-1}) as reported in the main text by:

195 $$MFSP = \frac{C}{\zeta F_{i=Ethanol}^{SK}} \#(23)$$

196 $$CF = \frac{1000 \, G}{3.6 \, \kappa_{i=Ethanol} F_{i=Ethanol}^{SK}} \#(24)$$

Reference

1. Sun, Q. *et al.* Selection of appropriate biogas upgrading technology-a review of biogas cleaning, upgrading and utilisation. *Renew. Sustain. Energy Rev.* **51**, 521–532 (2015).

2. Humbird, D. *et al. Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover.* http://www.osti.gov/scitech/biblio/1013269 (2011).

3. Davis, R. *et al. Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons: Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Catalytic Conversion of Sugars to Hydrocarbons.* NREL/TP--5100-62498, 1176746 http://www.osti.gov/servlets/purl/1176746/ (2015) doi:10.2172/1176746.

4. Davis, R. E. *et al. Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Coproducts: 2018 Biochemical Design Case Update; Biochemical Deconstruction and Conversion of Biomass to Fuels and Products via Integrated Biorefinery Pathways.* NREL/TP--5100-71949, 1483234 http://www.osti.gov/servlets/purl/1483234/ (2018) doi:10.2172/1483234.

5. Dutta, A. *et al. Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels.* http://www.nrel.gov/docs/fy15osti/62455.pdf (2015).

6. Huang, K., Fasahati, P. & Maravelias, C. T. System-Level Analysis of Lignin Valorization in Lignocellulosic Biorefineries. *iScience* **23**, 100751 (2020).

7. US EPA, O. RIN Trades and Price Information. https://www.epa.gov/fuels-registration-reporting-and-compliance-help/rin-trades-and-price-information (2018).

8. Alternative Fuels Data Center: Clean Fuel Production Credit. https://afdc.energy.gov/laws/13321.

9. Kim, B., Misra, S. & Maravelias, C. T. Lignocellulosic fuel and chemical co-production. *Joule* **7**, 2403–2407 (2023).

10. US Electricity Profile 2023. https://www.eia.gov/electricity/state/.

11. US EPA, O. Summary Data. https://www.epa.gov/egrid/summary-data (2020).

12. National Renewable Energy Laboratory/USLCI | LCA Collaboration Server. https://www.lcacommons.gov/lca-collaboration/National_Renewable_Energy_Laboratory/USLCI_Database_Public/datasets/Processes.