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Electronic Supplementary Information

Use of Ensiled Biomass Sorghum Increases Ionic Liquid Pretreatment Efficiency and Reduces Biofuel Production Cost and Carbon Footprint

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S1. Data inputs used to model ensiled and dry biomass sorghum bale supply systems

Table S1. Primary nutrients for biomass sorghum and their prices (the same parameters are used for dry and ensiled biomass supply system systems)

Parameter	Unit	μ	а	b	σ	Probability distribution
Nitrogen ^{1–5}	kg/ha	121.2 4	48.00	217.00	51.88	Triangular
Phosphorus ^{1,3,5}	kg/ha	23.89	9.30	67.25	16.74	Triangular
Potassium ^{1,3,5}	kg/ha	168.0 9	20.00	293.66	100.5 3	Triangular
Price of nitrogen ^{6–10}	\$/kg	1.06	0.60	1.40	0.34	Triangular
Price of phosphorus ^{6–}	\$/kg	1.01	0.82	1.20	0.15	Triangular
Price of potassium ^{6–10}	\$/kg	1.09	0.91	1.26	0.14	Triangular
Herbicides ^{11–13}	kg/ha	3.13	1.79	5.60	-	Triangular
Herbicides ^{11–14}	\$/ha	62.12	24.46	111.20	-	Triangular

Note: μ = average value; \mathbf{a} = minimum value; \mathbf{b} = maximum value; σ = standard deviation

Table S2. Operating data and purchasing price for forage harvester (for the ensiled biomass supply system)

Parameter	Unit	μ	а	b	σ	Probability distribution
Forage harvester						
Productivity ^{15–17}	t/h	31.67	26.33	49.22	10.45	Triangular
Field efficiency ^{15,16,18}	%	76.43	60.00	90.00	9.88	Triangular
Fuel consumption ¹⁶	L/h	61.61	28.62	104.15	26.85	Triangular
Labor rate ¹⁹	\$/h	19.36	12.62	29.81	6.82	Triangular
Wagon unloading time ^{15,16}	h	0.03	0.02	0.05	0.02	Triangular
Purchasing price ^{15,16,20–22}	\$/unit	230,570	179,334	259,725	30,710	Triangular
Repair and maintenance ^{15,16,18}	%	7.36	5.57	10.14	-	Triangular
Service life ^{15,16,18}	yr	4.50	4.00	5.00	-	Constant
Salvage value ^{15,16,18}	%	18.60	15.00	25.00	-	Constant
Material loss ^{15,17}	%	6.00	2.00	10.00	-	Triangular

Note: μ = average value; a = minimum value; b = maximum value; σ = standard deviation

Table S3. Operating data and purchasing price for windrower and windrow turner (only for dry biomass supply system)

Parameter	Unit	μ	а	b	σ	Probability distribution
Windrower						
Productivity ^{15,16,23}	t/h	32.39	19.63	54.14	13.38	Triangular
Field efficiency ^{15,16,23}	%	75.00	50.00	90.00	12.91	Triangular
Fuel consumption ^{15,16,23}	L/h	25.06	18.90	34.10	6.87	Triangular
Labor rate ¹⁹	\$/h	19.36	12.62	29.81	6.82	Triangular
Purchasing price ^{15,16,23}	\$/unit	48,691	23,000	83,096	23,234	Triangular
Repair and maintenance ^{15,16}	%	27.50	7.50	48.00	20.25	Triangular
Service life ^{15,16}	yr	4.50	4.00	5.00	0.71	Constant
Salvage value ^{15,16}	%	19.72	15.00	25.00	4.12	Constant
Windrow turner/raking						
Productivity ^{15,16}	t/h	64.78	2.64	108.27	26.76	Triangular
Field efficiency ^{15,16}	%	75.00	50.00	90.00	12.91	Triangular
Fuel consumption ^{15,16}	L/h	9.12	7.56	11.34	1.97	Triangular
Labor rate ¹⁹	\$/h	19.36	12.62	29.81	6.82	Triangular
Purchasing price per unit ^{15,16}	\$	37,876	37,103	38,649	1,093	Triangular
Repair and maintenance ^{15,16}	%	7.36	5.57	10.14	2.00	Triangular
Service life ^{15,16}	yr	6.25	5.00	7.50	1.77	Constant
Salvage value ^{15,16}	%	12.30	5.00	24.00	8.19	Constant

Note: μ = average value; a = minimum value; b = maximum value; σ = standard deviation

Table S4. Operating data and purchasing price of baler and stacker (Only for dry biomass supply system)

Parameter	Unit	μ	a	b	σ	Probability distribution
Baler ^{16,23,24}						
Productivity	t/h	25.91	20.00	43.31	10.70	Triangular
Field efficiency	%	66.29	35.00	90.00	19.36	Triangular
Fuel consumption	L/h	33.50	18.90	53.00	12.84	Triangular
Labor rate	\$/h	20.11	12.62	29.81	7.18	Triangular
Consumable: string	m/bale	38.00	38.00	38.00	-	Constant
Cost of consumable string	\$/m	0.02	0.02	0.02	0.00	Constant
Purchasing price	\$/unit	109,531	87,700	135,000	17,986	Triangular
Repair and maintenance	%	20.00	5.00	35.00	21.21	Triangular
Service life	year	6.00	5.00	7.00	1.41	Constant
Salvage value	%	22.50	20.00	25.00	3.54	Constant
Stacker ^{16,23,24}						
Productivity	bales/h	65.00	50.00	80.00	10.64	Triangular
Field efficiency	%	87.00	70.00	97.00	10.20	Triangular
Fuel consumption	L/h	21.17	8.47	37.90	12.00	Triangular
Labor rate	\$/h	20.11	12.62	29.81	7.18	Triangular
Purchasing price	\$/unit	79,967	70,000	90,000	10,000	Triangular
Repair and maintenance	%	26.17	3.33	49.00	32.29	Triangular
Service life	year	5.00	5.00	5.00	-	Constant
Salvage value	%	10.00	5.00	15.00	7.07	Constant

Note: μ = average value; a = minimum value; b = maximum value; σ = standard deviation

S1.1 Transportation of chopped biomass and bale

The harvested biomass in the form of chopped biomass and bales are transported directly from the field to the biorefinery. This transportation operation includes loading at the field edge, transportation via truck, and unloading at the biorefinery. The chopped biomass is directly loaded on the truck by the forage harvester, therefore, the loading operation at the field is excluded. However, all the loading, transportation, and unloading operations associated with the feedstock transportation are included to transport bales, which are consistent with previous studies. ^{23,24} Briefly, squeeze bale loader is used to load and unload the bales. A group of people conducts these loading and unloading operations. For each group, two squeeze bale loaders (one at each end) and 4 trucks²⁵ are assigned. Each truck can carry as much as 36 bales/trip due to the size limit. We consider a box truck with a capacity of 133.8 m³ to transport chopped biomass¹⁶ where the maximum payload is assumed to be 22.7 t. Table S5 summarizes the operating data associated with feedstock transportation. The detailed methods for estimation of resources and cost for feedstock transportation are available elsewhere. ^{24,26,27}

Table S5. Operating data associated with the feedstock transportation operation

Parameter	Unit	μ	а	b	σ	Probability distribution	
Truck							
Purchasing price ^{16,28}	\$/unit	140,000	130,000	150,000	-	Triangular	
Labor cost ¹⁹	\$/h	20.83	12.94	30.36	6.95	Triangular	
Fuel consumption ²⁴	L/km	0.43	0.35	0.50	0.06	Triangular	
Diesel price ²⁹	\$/L	0.88	0.61	1.05	0.18	Lognormal	
Loader for bale							
Purchasing price16	\$/unit	30,000	20,000	40,000	-	Triangular	
Labor cost ¹⁹	\$/h	19.36	12.62	29.81	6.82	Triangular	
Fuel consumption ²⁴	L/h	20.80	17.00	24.60	5.70	Triangular	
Loading time ²⁴	h	0.63	0.33	0.95	0.31	Triangular	
Unloading time ^{ϕ24}	h	0.49	0.17	1.49	0.58	Triangular	
Storage or biorefinery transport for chopped biomass and bale							
Working days ³⁰	days/yr	31.54	15.00	75.00	14.59	Triangular	
Working hours $^{\lambda}$	h/day	16.00	8.00	24.00	8.00	Triangular	

Note: μ = average value; a = minimum value; b = maximum value; σ = standard deviation

S1.2 Feedstock storage at the biorefinery

Different storage methods for the chopped biomass and bale are used at the biorefinery. The chopped biomass is ensiled in a bunker silo, which is covered by the tarp. This ensiling process creates an anaerobic environment, which prevents degradation of the quality of biomass. Bale (contains <20% moisture) are stored in open space under the tarp. Gravels are laid on the floor to protect bales and module from moisture seepage from ground. Detailed methods to estimate the storage cost is provided in the previous studies. 18,23,24

S2. Determination of minimum selling price and greenhouse gas footprint

The capital and operating costs obtained from the process model are used to determine the minimum price of the selected biofuels considering the internal rate of return (IRR) after taxes of 10%, plant lifetime of 30 years, plant operating hours of 7920 h (330 days/year and 24 h/day), and income tax of 35%.²² Other economic evaluation parameters are consistent with previous technoeconomic studies.^{20,22} On the other hand, the material and energy data obtained from the process model are used to quantify the carbon footprint. We use previously developed life cycle assessment model, which computes the GHG emissions considering the input-output matrix for all relevant direct and indirect inputs/outputs and the GHG impact vectors gathered from widely used LCA databases, including GREET developed by Argonne National Laboratory, and U.S. Life Cycle Inventory Database.²¹ The modeled biorefinery generates sufficient process heat and

^oThe same unloading (includes unloading and waiting time) time is considered for the chopped biomass.

 $^{^{\}lambda}$ Assumed based on the current harvesting practices of biomass sorghum.

electricity to meet the facility requirement. The GHG emissions credit from onsite electricity is determined considering the displacement of the same amount of grid electricity (U.S. electricity mix). We consider higher heating values of ethanol the functional unit of 1 MJ.

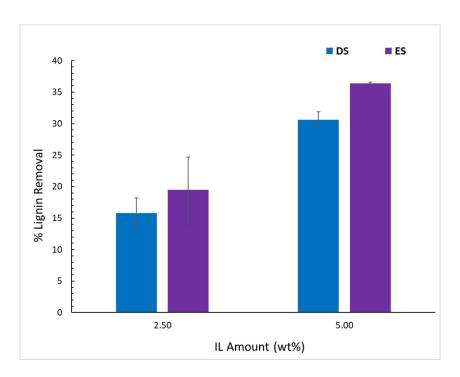


Figure S1. Lignin removal of ES and DS biomass during the IL pretreatment. The IL loading rates are 2.5, and 5 wt% based on the whole slurry.

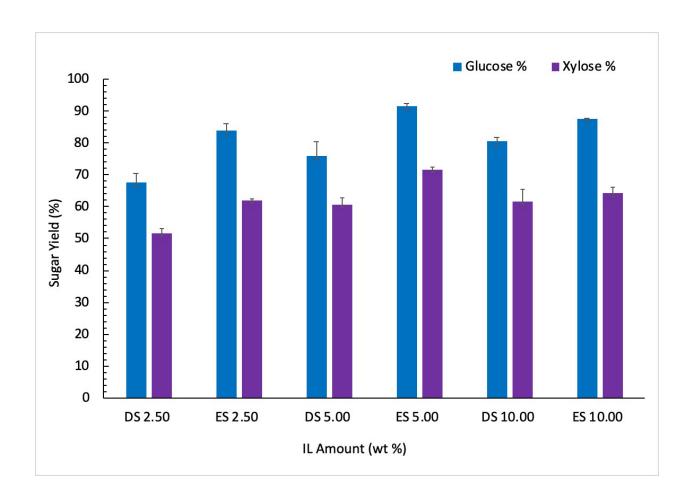


Figure S2. Glucose and xylose yields obtained by performing a one-pot IL process utilizing the ES and DS biomass. The IL loading rates are 2.5, 5, and 10 wt% based on the whole slurry.

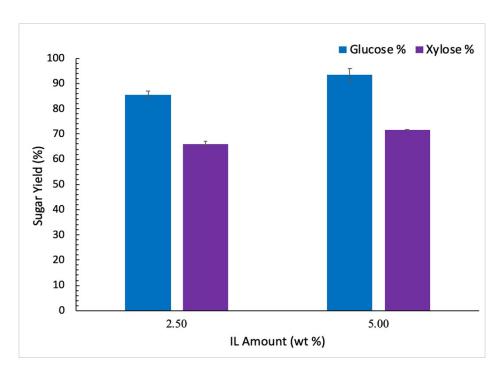


Figure S3. Glucose and xylose yields obtained by performing a one-pot IL process utilizing the ES in Parr reactor at 140 °C. The IL loading rates are 2.5 and 5 wt% based on the whole slurry.

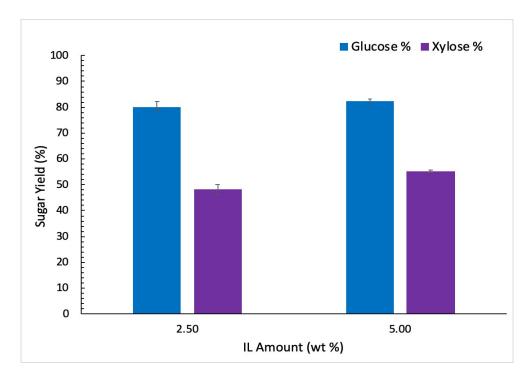


Figure S4. Glucose and xylose yields obtained by performing a one-pot IL process of ES at 95 °C. The IL loading rates are 2.5 and 5 wt% based on the whole slurry.

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