SUPPORTING INFORMATION

The supporting information consists of 5 pages, including cover page, containing 3 figures and 7 tables.

Environmental and Cost Evaluation of Lignocellulosic Path to Sustainable Aviation Fuel

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SUPPORTING FIGURES

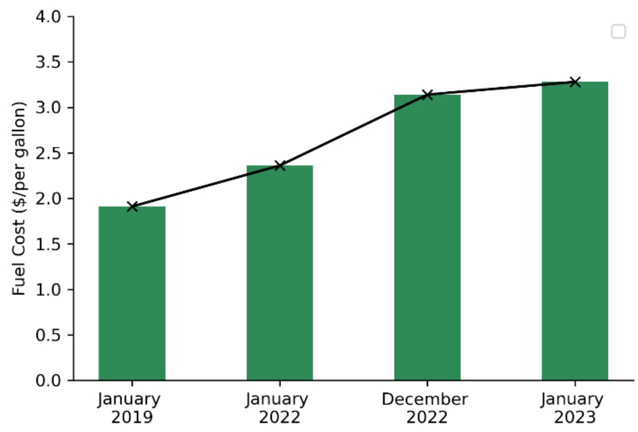


Figure S1. Petroleum Jet Fuel price January 2019-2023 [1]

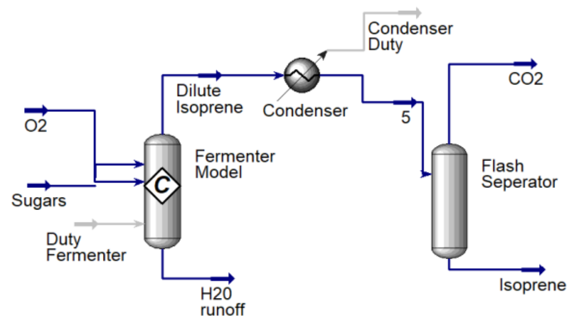


Figure S2. PFD of UniSim Fermentation Modeling Area*

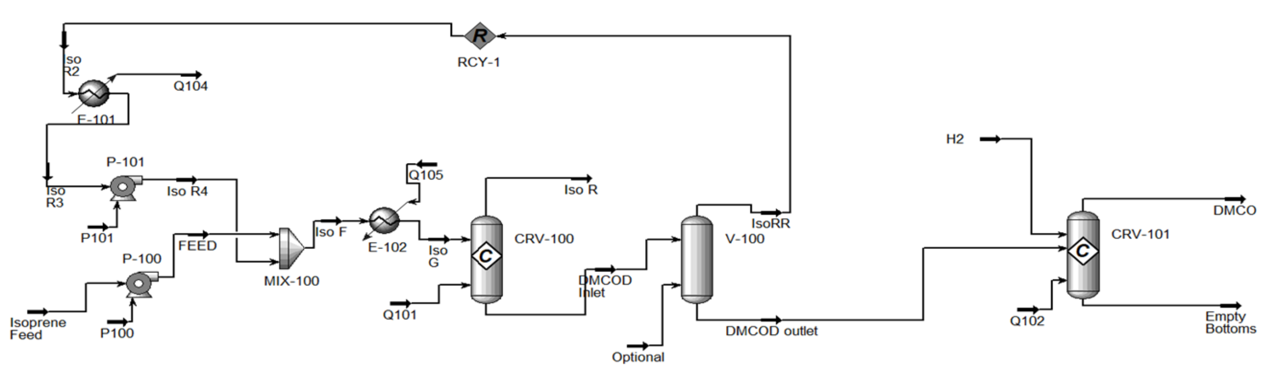


Figure S3. PFD of Catalytic Upgrading and Hydrogenation Modeling Area*

***The UniSim files can be made available on request**

SUPPORTING TABLES

Table S1. Energy requirements for conversion of fermentable sugars in biomass to DMCO

Fermentation Heat Duty	1708	kJ/kg of isoprene produced
Condenser Duty	87.3	kJ/kg of isoprene recovered
Recirculation pumps	0.001	kJ/s per pump
Dimerization	-3413.9	kJ/kg isoprene
Dehydration reactor duty	1.5	kJ/kg of MBE fed
Hydrogenation pre-heat	0.4	kJ/kg isoprene
Hydrogenation Duty	385.5	kJ/kg isoprene

Table S2. Life cycle inventory input data for corn stover based DMCO (per 1 kg isoprene)

Item	Amount	Unit	Source and assumptions
Upstream			Emissions due to corn stover harvest and replacement of nutrients are allocated to the corn stover and emissions from nutrient inputs for crop production are allocated to the corn crop
Feedstock input	6.5	kg	Calculated based on our model and conversions of different stages
Feedstock yield	9.7	ton/ha/yr	Spatari et al.[2]
Collection	1.7	MJ	Using data from Spatari et al.[2] and Pourhashem et al.[3]
Nutrient replacement	N 33 P 11.9 K 60.7	g	Based on GREET results from Spatari et al.[2] for nutrient replacement due to corn stover removal
N_2O emissions	Direct: 0.3 Indirect: 0.4	g	Based on DayCent model[4] results from Adler et al.[5] and Pourhashem et al.[3]
Change in soil carbon	1.2	kg CO_2	Based on DayCent model[4] results from Adler et al.[5] and Pourhashem et al.[3]
Diesel for transportation	30.7	ml	Assuming 80 km transportation distance including the return trip and using diesel powered truck from the USLCI database in SimaPro[6] software
Biorefinery			
Fermentation energy	898.9	KJ	Calculated required amount of energy and chemicals using UniSim[7] simulation and using Ecoinvent database[8] for life cycle impact assessment
Heat Duty Fermenter	7.88	KJ	Energy needed to raise the Temperature of reactor, including 1L of water. 2.67g isoprene/ 3.74 g of sugars –UniSim Simulation Model
Recirculation Pumps	0.001	kJ/s	Fermenter recirculation pumps per pump [9]
Air Compressor	0.004	kWh	UniSim Simulation Model 1.247 kJ/hr /3600 to convert to kW then * 2.86hrs for 1kg isoprene
Separation cooling energy	-1938.8	KJ	UniSim Simulation Model
Separation heating energy	2068.9	KJ	UniSim Simulation Model
Dimerization energy	-3413.9	KJ	UniSim Simulation Model
Hydrogenation energy	385.5	KJ	UniSim Simulation Model
Surplus electricity	8742	KJ	Difference between the total electricity generated onsite from lignin combustion in the boiler and the electricity required by the bioplant; assumed to replace from the MRO electricity grid

Table S3. Cost contribution of various sections to the Minimum Fuel selling price (MFSP) for the DMCO and electricity. All cost in $/L DMCO.

AREA	Capital Recovery Charge	Raw Materials & Waste	Process Electricity	Grid Electricity	Total Plant Electricity	Fixed Costs	Area Totals
Feedstock and Handling	$0.000	$0.364	$0.000	$0.000	$0.000	$0.000	$0.364
Pretreatment and Conditioning	$0.055	$0.048	$0.014	$0.000	$0.000	$0.012	$0.129
Enzymatic Hydrolysis and Fermentation	$0.035	$0.008	$0.007	$0.000	$0.000	$0.007	$0.057
Cellulase Enzyme Production	$0.021	$0.306	$0.013	$0.000	$0.000	$0.004	$0.345
Distillation and Solids Recovery	$0.020	$0.000	$0.005	$0.000	$0.000	$0.004	$0.030
Wastewater Treatment	$0.075	$0.027	$0.018	$0.000	$0.000	$0.016	$0.136
Storage	$0.008	$0.000	$0.000	$0.000	$0.000	$0.002	$0.010
Boiler and Turbogenerator	$0.110	$0.029	$0.003	-$0.034	-$0.069	$0.023	$0.063
Utilities	$0.012	$0.004	$0.008	$0.000	$0.000	$0.002	$0.025
NET SUMMATION	$0.336	$0.786	$0.069	-$0.034	-$0.069	$0.070	$1.159

Table S4. CAPEX in year 2018 with changes to NREL's Model 2015 according to process steps. All cost in USD$.

Area	EQUIPMENT TITLE	DESCRIPTION	$	Year of Quote	Purch Cost in Base Yr	Scaling Val	Units	Scaling Exp	Inst Factor	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year	Remarks
Fermentation	ISOPRENE FERMENTER (Bioconversion reactor)	Total Vessel Volume: 3785 m^3	$7,792,000	2017	$7,792,000	1	ea	1.00	0.5	$7,792,000	$8,280,802	$4,140,401	UniSim Model and Humbird et al. 2017[11]
	ISOPRENE CONDENSER	Shell and tube	$718,084	2017	$718,084	1	ea	1.00	1.5	$718,084	$763,131	$1,144,696	UniSim model and Excel costing [10]
	Isoprene Transfer Pump	2153 GPM, 171 FT TDH	$214,400	2010	$214,400	18833	kg/hr	0.80	2.3	$417,452	$457,091	$1,051,309	Goulds [12]
	Fermenter Air Compressor Package	8000 SCFM @ 16 psig	$350,000	2009	$350,000	33168	kg/hr	0.60	1.6	$346,282	$400,158	$640,253	Dresser Roots [12]
Dimerization	Dimerziation Reactor		$3,485,301	2017			kg/hr	1.00	1.5	$3,485,301	$3,703,939	$5,555,908	UniSim model and Excel costing [10]
	Hydrogen recovery unit		$993,634	2018			kg/hr	1.00	1.5	$993,634	$993,634	$1,490,451	Baral et al. 2021[13]
	Catalyst recovery unit						kg/hr	1.00	1.5	$0		$0	Assumed in OPEX costs
	Flash seperator		$43,129	2018			kg/hr	1.00	1.5	$43,129	$43,129	$64,693	Excel costing[10]
Hydrogenation	Hydrogenation reactor	(Q3 FY17 milestone), base PF=2.5,208 BBL/hr	$4,168,568	2011	$4,168,568	32895	L/hr	0.70	2.0	$2,194,971	$2,194,971	$4,389,943	UniSim model and Excel costing [10]
	Hydrogen compressor	25.3 kW	$87,283	2018			kg/hr	1.00	1.5	$87,283	$87,283	$130,924	Excel Costing [10]

Table S5. Variable OPEX year 2018 USD (indexed) with changes to NREL's Model 2015 according to process steps.

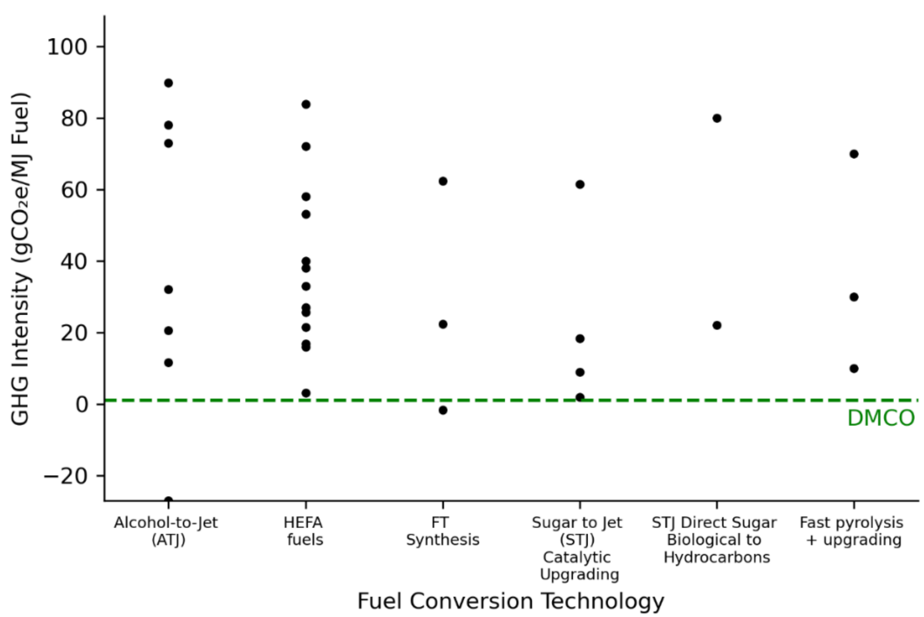
Area	Raw Material	kg/hr	lb/hr	Quoted Price (cents / ton)	Year of Price Quote	2018 Cost ($ / ton)	2018 Cost ($/lb)	$/hour	MM$/yr (2018)	Cents/Gallon DMCO (2018)	Remarks - Cost reference
Feedstock and Handling	Feedstock	104,167	229,688	5701	2018	57.01	0.03	6,547.01	55.06	134.77	
Pretreatment and Conditioning	Sulfuric Acid, 93%	1,500	3,308	9000	2009	116.18	0.06	192.14	1.62	3.96	Basic Chemical, Omaha via HGI
	Ammonia	1,051	2,317	45000	2009	580.92	0.29	673.01	5.66	13.85	Terra Industries via HGI, anhydrous, delivery to Iowa
Enzymatic Hydrolysis and Fermentation	CSL	580	1,278	5700	2009	73.58	0.04	47.02	0.40	0.97	Corn Products via HGI
	DAP	19	42	99000	2009	1278.02	0.64	26.86	0.23	0.55	Ronas Chemicals via HGI
	Sorbitol	44	98	113000	2009	1458.75	0.73	71.36	0.60	1.47	Coast Southwest via HGI
Cellulase Enzyme Production	Purchased Enzyme	0	0	0	2018	0.00	0.00	0.00	0.00	0.00	Not considered in NREL Davis et al. 2015
	Glucose	2,418	5,332	58220	2009	751.58	0.38	2,003.56	16.85	41.24	USDA
	Tryptone	164	363	5700	2009	73.58	0.04	13.34	0.11	0.27	Corn Products via HGI
	Ammonia	115	254	45000	2009	580.92	0.29	73.64	0.62	1.52	Terra Industries via HGI, anhydrous, delivery to Iowa
	Host nutrients	67	149	74530	2007	1063.88	0.53	79.00	0.66	1.63	SRI CEH
Catalytic conversion, upgrading and storage	Dimerization catalyst	24	54	930582	CatCost NREL	9305.82	4.65	251.19	2.11	5.17	Baral et al 2021 ($10.26 $/kg - 0.13%wt) and Isoprene feed (18833kg/hr) dual pathway
	Hydrogenation catalyst	81	179	1315150	CatCost NREL	13151.50	6.58	1,174.20	9.88	24.17	Baral et al 2021 ($14.5 $/kg - 0.43%wt) and DMCOD feed (18833kg/hr) dual pathway
	Hydrogen production	417	kg/h	4.49	$/kg			1,870.83	15.73	38.51	Title: Hydrogen Production Cost Using Low-Cost Natural Gas Originator: Sara Dillich, Todd Ramsden & Marc Melaina
	Hydrogen recovery cost	69	kmol/h	0.50	$/kmol			34.43	0.29	0.71	Minimum H2 req for dry feed
	Sulfur Dioxide	16	36	25400	2005	393.54	0.20	7.12	0.06	0.15	Hydrogen management in refineries Rabie and excel Hydrogen calculation
Wastewater Treatment	Caustic (as pure)	2,252	4,966	15000	2009	193.64	0.10	480.77	4.04	9.90	SRI CEH
Combustor, boiler, and turbo-generator	Boiler Chems	0	1	280000	1991	6469.43	3.23	1.76	0.01	0.04	
	FGD Lime	894	1,972	20000	2009	258.19	0.13	254.60	2.14	5.24	
	Feedstock	0	0	5701	2018	57.01	0.03	0.00	0.00	0.00	Set in Cell I20
Utilities	Cooling Tower Chems	2	5	200000	1999	3877.09	1.94	10.19	0.09	0.21	
	Makeup Water	147,136	324,435	20	2004	0.34	0.00	54.40	0.46	1.12	Peters & Timmerhaus
Waste Streams	Disposal of Ash	5,724	12,622	1820	1993	41.20	0.02	259.99	2.19	5.35	
By-Products and Credits	Grid Electricity	12,814	kW	by year	2018	$/kWh	0.04	572.02	4.81	11.77	
	Area 100 Electricity	859	kW	by year	2018	$/kWh	0.04	38.37	0.32	0.79	
	Lubricant	0	kg/h	1.2000	$/kg			0.00	0.00	0.00	
	Total Variable Operating Costs							13,461.65	113.67	278.22	

Table S6. Fixed OPEX in year 2018 with changes to NREL's Model 2015 according to process steps. All cost in USD$.

	Position	**Salary**	**Year of salary quote**	**2018 Salary**	**# Required**	**Total**	**2018 Cost USD$**
Labor & Supervision	Plant Manager	147000	2009	184,366	1	147,000	184,366
	Plant Engineer	70000	2009	87,793	2	140,000	175,586
	Maintenance Supervisor	57000	2009	71,489	1	57,000	71,489
	Maintenance Tech	40000	2009	50,167	12	480,000	602,010
	Lab Manager	56000	2009	70,234	1	56,000	70,234
	Lab Technician	40000	2009	50,167	2	80,000	100,335
	Lab Tech-Enzyme	40000	2009	50,167	2	80,000	100,335
	Shift Supervisor	48000	2009	60,201	4	192,000	240,804
	Shift Operators	40000	2009	50,167	20	800,000	1,003,350
	Shift Oper-Enzyme	40000	2009	50,167	8	320,000	401,340
	Yard Employees	28000	2009	35,117	4	112,000	140,469
	Clerks & Secretaries	36000	2009	45,151	3	108,000	135,452
	Total Salaries					2,572,000	3,225,769
	Labor Burden (90%)					2,314,800	2,903,193
Other Overhead	Maintenance	3.0%	of ISBL				2,699,254
	Property Insur. & Tax	0.7%	of FCI				3,067,839
	Total Fixed Operating Costs						11,896,055

Table S7. GHG intensity of DMCO as compared to Fuel Conversion Technology pathways: ATJ, HEFA Fuels, FT Synthesis, STJ Catalytic Upgrading, STJ Direct Sugar Biological to Hydrocarbons and Fast Pyrolysis.

#	Fuel Conversion Technology	Feedstocks	Fuel Density (g/ml)	GHG Intensity (gCO2/MJ)	References
1	Alcohol-to-Jet (ATJ)	Starch crops	0.59 to 0.79	-27 to 78	Han (2017) [14], Gollakota (2021)[15]
		Switchgrass	0.59 to 0.79	12 to 90	Staples (2014)[16]
		Poplar	0.59 to 0.79	32 to 73	Budsberg(2016)[17]
		Sugarcane, molasses	0.59 to 0.79	-27 to 21	Tanzil (2022)[18] Staples et al (2014)[16]
2	HEFA fuels	Microalgae oil	0.77 to 0.84	27 to 38	Cox (2014)[19]
		Camelina oil	0.77 to 0.84	3 to 53	Stratton (2011)[20] Jong (2017)[21]
		Jatropha oil	0.77 to 0.84	33 to 40	Bailis (2010)[22]
		Waste oils	0.77 to 0.84	17 to 21	Seber (2014)[23]
		Animal fats	0.77 to 0.84	26 to 84	Seber (2014)[23]
3	FT Synthesis	Camelina oil	0.79 to 0.81	22	Shonnard (2010)[24]
		Lignocellulose biomass, municipal waste	0.79 to 0.81	-2 to 62	Jong (2017)[21] Suresh (2018)[25]
4	Sugar to Jet (STJ) Catalytic Upgrading	Lignocellulose biomass	0.77 to 0.84	18 to 61	Riazi (2018)[26] Baral (2021)[13]
5	STJ Direct Sugar Biological to Hydrocarbons	Sugarcane, starch crops, lignocellulose biomass	0.77 to 0.84	22 to 80	Han (2017)[14] Cox (2014)[19]
6	Fast pyrolysis + upgrading	Equine waste	Up to 0.91	10 to 70	Sorunmu (2017)[27] Elkasabi (2020)[28] Fitriasari (2023)[29]



Sample calculation for jet-fuel credit

Calculate the GHG emissions per liter of fuel for jet A fuel:

GHG emissions per liter of jet fuel = 89 gCO_2/MJ x 33 MJ/L ≈ 2950 gCO_2/L
Equivalent GHG emissions per liter of DMCO = 89 gCO_2/MJ x 36.3 MJ/L ≈ 3230 gCO_2/L

Savings in GHG emissions per liter = 2945.9 gCO_2/L – 3230.7 gCO_2/L ≈ -284.8 gCO_2/L

Savings in GHG emissions per MJ DMCO = $\frac{-284.8\ \mathrm{gCO_2/L}}{36.2\ \mathrm{MJ/L}}$ = 7.9

Fuel Type	**Net Heat of Combustion (MJ/L)**	**GHG Emissions (gCO2/L)**	**Difference in GHG Emissions (gCO2/L)**	**Savings per MJ (gCO2/MJ)**
Conventional Jet Fuel (89 gCO_2 /MJ)	33.1	2945.9	-	-
DMCO (eq.)	36.2	3230.7	284.8	7.9

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