Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Techno-economic analysis and life-cycle greenhouse gas mitigation cost of five routes to bio-jet fuel blendstocks

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Electronic Supporting information (ESI)

S1. Additional information

S1.1 Sorghum biomass feedstocks and ionic liquid -based deconstruction processes

The cost of sugar is largely dependent on biomass feedstock price at the biorefinery gate. Among lignocellulosic feedstocks, biomass sorghum is one of the more promising near-term feedstocks for biofuel production due to its high yield of up to 27.57 ± 6.81 metric ton (t)/ha,[1–7] its natural drought tolerance,[1] and farmers' familiarity with it as a feed crop. The U.S. currently utilizes about 2.5 million ha (6.69 million acres) of land (1.7 % of the total cropland of U.S.) for sorghum production,[5] although this fraction will likely increase[1] if sorghum becomes a widely-used feedstock for cellulosic biofuel production.

The sugar production cost is dependent on the selection of pretreatment process. Pretreatment is an essential step to break up the recalcitrant structure of lignocellulosic biomass and facilitate the conversion of cellulose and hemicellulose into its constituent six- and five-carbon sugars. There are several physical, chemical (acidic and alkaline), and biological pretreatment processes available.[8–10] Among these pretreatment technologies, dilute sulfuric acid pretreatment technology is already commercialized; however, it produces microbial compounds inhibitory to microbes from polysaccharides such as weak acids, furan derivatives, and phenolic compounds[11] and requires a detoxification step[12] before the downstream conversion processes. Additionally, while dilute sulfuric acid solubilizes the hemicelluloses, the lignin fraction of biomass remains on the surface of crystalline cellulose, which reduces enzyme-accessible area and resulting overall sugar yield.[13] In this paper, we focus on ionic liquid (IL) pretreatment, a promising alternative to the conventional pretreatment approaches, which can be used effectively for a wide range of lignocellulosic biomass types such as agricultural residues, energy crops, forest residues, and heterogeneous blends.[8,14–17]

The main economic barrier of IL pretreatment technology is the production cost of the IL itself and the resulting need to achieve a near-100% recycling rate,[18,19] which can be addressed by using cheaper ionic liquids (such as choline-based, and protic ILs), and an efficient IL recovery process.[20–23] This study considers two promising ILs: cholinium lysinate ([Ch][Lys], a choline-based IL) and ethanolamine acetate ([EOA][OAc], a protic IL) based on their several advantages (i) nontoxic to enzyme and bioconversion microorganism up to 10 and 2.5 wt%, respectively in the case of [EOA][OAc], (ii) pH-compatible with downstream operations ([EOA][OAc] only), (iii) allow for high solids loading of up to 40 wt% during pretreatment, and (iv) low production costs compared to a widely studied IL (1-ethyl--3-methylimidazolium acetate).[22] Because of their bio-compatibility, these ILs enable integrated high-gravity/one-pot biofuel production systems, which dramatically lower costs relative to the previous state-of-technology, that uses an intensive water-wash process, by avoiding costly washing and separation steps.[20]

S1.2 Feedstock handling and preprocessing

Our lignocellulosic biomass feedstock handling and the preprocessing system was developed in line with the techno-economic models developed by NREL.[12,24] This system includes a truck scale, truck dumper, truck dumper hopper, dust collection, and storage system. In addition to these, a grinding unit was added to reduce the size of feedstock if the feedstock is transported as bales. Belt or screw conveyors were used to move the biomass from one piece of process equipment to another. Throughput and the required energy of each process equipment associated with handling and preprocessing were gathered form previous studies[12,24] and assigned in the process model developed in this study. This unit supplies the preprocessed feedstock to the pretreatment unit.

S1.3 Methods for GHG emissions calculation

This study quantifies and compare the equivalent amount of CO_2 emissions for five potential jet fuel molecules including limonane via limonene, limonane via 1,8-cineole, RJ-4, bisabolane, and epi-isozizaane. The theoretically estimated lower and higher heating values are summarized in Table S1. The system boundary includes biomass sorghum feedstock supply logistics, and downstream jet fuel production processes (Fig. 2). Additionally, we considered GHG emissions from land use change.[1,25] The net GHG emissions from land use change is taken from the best-available literature, and includes net emissions associated with the loss of top soil carbon and existing vegetation when land is converted for sorghum cultivation,[26] carbon sequestration from accumulation of below-ground biomass,[27] and the emissions associated with indirect land use change.[28] The soil carbon sequestration potential of biomass sorghum reported in the DOE Billion-Ton study is striking in that it is larger than other bioenergy crops, including perennial grasses.[27] However, the soil organic carbon gain with biomass sorghum farming in cropland/pasture land presented in the DOE Billion-Ton study[27] is based on only a limited number of counties and there are not many supporting studies in the scientific literature, therefore, the soil carbon sequestration potential of biomass sorghum requires further analysis. We accounted the variability present in the data inputs (-3.83 to -0.16 tCO_{2e}/ha/year[26,27]) and presented the resulted uncertainty with error bars. The indirect land use change values are also in need of further study and refinement in future studies, as the only literature values available are based on grain sorghum rather than forage/biomass sorghum. This issue is further complicated because some sorghum types are considered “all-purpose” and may be used for either grain or silage. The estimated average value for the indirect land use changes based on grain sorghum is 0.79 tCO_{2e}/ha/year.[28] Consistent with previous study,[26] this study amortizes land use changes over 30 years.

To estimate direct and indirect emissions not related to land use change, we develop mass and energy balances based on best estimates for how biomass sorghum would be handled in bioenergy systems. The sorghum biomass feedstock supply logistics system encompasses nutrient replacement, harvesting, collection at the field edge, transportation to the biorefinery and outdoor storage next to the biorefinery. We consider biorefinery utilizes dry biomass sorghum feedstock of 1814.4 metric ton (t)/day (2000 dry ton/day) for all the 60 different scenarios. However, for the optimal condition, along with other optimal process conditions (S8) sorghum biomass utilization rate of 2721.5 t/day (3000 dry ton/day) is considered to take advantage of the economy of scale. The required biomass feedstock can be collected within the feedstock supply radius of <80 km if the biomass sorghum growing land is at least 2% of the total land around the biorefinery and the dry matter loss of the entire supply chain is 20 wt% or less. Additionally, the downstream processes include feedstock handling, IL pretreatment, hydrolysis and bioconversion, recovery and separation, hydrogenation, wastewater treatment, and onsite energy generation.

The detailed process models were developed in the modeling software SuperPro Designer (SPD)-V10. Fig. 2 presents a brief overview of the process model including the required process chemicals and utilities. Table S2 summarizes the major inputs to the process models developed in this study and their probability distributions. We develop an LCA model by using Python. The mass and energy balances that were calculated from the SPD were the main inputs of the LCA modeling. These data are presented in Tables S3-S8. A hybrid lifecycle assessment approach that utilizes process-based and input-output (IO) based LCA was used to quantify the environmental impacts of all processes. We developed an input-output vector for all processes that take place in our system and followed a similar methodology as previously employed by Neupane et al.[29] to compute the GHG emissions. The previous study[29] has provided the impact vectors to determine GHG emissions, which is available for download in excel format. The upstream life-cycle inventory data were collected from widely used LCA databases[30–32] and previous[29] literature. Energy and emissions associated with buildings and process equipment were excluded in the analysis as these different jet fuel production routes considered in this study require the similar level of process equipment and facilities. On the other hand, process energy and emissions associated with the production of the required process chemicals, along with chilled water and process steam were included in the analysis and their environmental impacts were quantified. In the current LCA analysis the current US electricity mix is assumed for all the direct electricity consumption impacts. These considerations provide the total GHG emissions of each process. Electricity and process steam generated from the onsite energy generation section (Fig. 2) are assigned as credits then the net GHG emissions is estimated. Global Warming Potential (GWP) was evaluated considering the emissions contributed by the common greenhouse gases including CO_2, CH_4, and N_2O using the 100-year horizon GWP factors of 1, 25 and 298 for CO_2, CH_4, and N_2O, respectively.

Table S1. Lower and higher heating values and density of the jet fuel molecules

Molecule	Heating value (MJ/kg)		Density (kg/L)
	LHV	HHV	
Limonane#	**43.41**	**46.32**	0.804[a]
RJ-4#	42.59[b]	**45.06[#,b]**	0.92[b]
Bisabolane#	**43.76**	**46.66**	0.814 [b]
Epi-isozizaane#	**42.33**	**44.89**	0.929 [b]
Jet A[33,34]	42.80	46.20	0.81

#Theoretically estimated values

[a]*https://pubchem.ncbi.nlm.nih.gov/compound/limonane via 1,8 cineole#section=Solubility*

[b]*These densities are experimentally determined at Naval Air Warfare Center, Weapons Division, and obtained through personal communication with Benjamin G. Harvey.*

Table S2. Input parameters and their probability distributions

Parameters	Units	Average	Minimum	Maximum	Standard deviation	Probability distribution
Cost of sorghum biomass[a]	$/t-dry	86.1	60.00	150	20.00	Lognormal
Sorghum biomass composition[3,7,38–43]						
Acetate	wt%	2.20	0.90	2.90		Constant
Ash	wt%	7.70	2.20	10.94	3.49	Lognormal
Cellulose	wt%	35.80	20.50	44.02	5.31	Lognormal
Hemicellulose	wt%	22.92	14.50	29.79	3.80	Lognormal
Lignin	wt%	16.52	9.89	20.29	2.70	Lognormal
Proteins	wt%	4.39	3.88	5.16	0.68	Constant
IL Pretreatment						
Solid loading rate[12,20,22]	wt%	30.00	20.00	40.00		Triangular
IL loading rate[20]	kg/kg-biomass	0.29	0.25	0.35		Triangular
IL-cost for [Ch][Lys] [20,29]	$/kg	2.00	1.43	5.00		Triangular
IL-cost for [EOA][OAc] [20,29]	$/kg	1.43	1	5		Triangular
Sulfuric acid loading[20,29]	kg-/kg-IL	0.16	0.15	0.17		Triangular
Sulfuric acid price[12,24,44]	$/kg	0.14	0.03	0.28	0.11	Triangular
Lignin to soluble lignin[20,29]	wt%	65.00	60	70		Constant
Pretreatment time [20,29]	h	3.00	2.5	3.4		Triangular
Enzymatic hydrolysis[20,22,29]						
Enzyme loading rate	mg/g-glucan	20.00	7	20		Uniform
Initial solid loading rate	wt%	20.00	20	30		Uniform
Cellulose to glucose for [Ch][Lys]	wt%	84.00	84	95		Uniform
Xylan to xylose for [Ch][Lys]	wt%	80.00	75	90		Uniform
Cellulose to glucose for [EOA][OAc]	wt%	80.00	75	90		Uniform
Xylan to xylose for [EOA][OAc]	wt%	75.00	70	90		Uniform
Hydrolysis time	h	48.00	36	72		Triangular
Enzyme price	$/kg-protein	5.00	4	6		Triangular

Contd.

Table S2. Input parameters and their probability distributions (Contd.)

Parameters	Units	Average	Minimum	Maximum	Standard deviation	Probability distribution
Bioconversion						
Aeration rate (aerobic) [45–47]	VVM	1.00	1.00	2.00		Triangular
Aeration rate (micro-aerobic) [45,46,48,49]	VVM	0.5	0.2	1.5		Triangular
Power consumption (aerobic) [50]	kW/m^3	3.00	2.00	5.00		Triangular
Power consumption (micro-aerobic) [50]	kW/m^3	0.35	0.2	0.6		Triangular
Power dissipation to heat (aerobic) [50,51]	%	80.00	70.00	100.00		Triangular
Power dissipation to heat (micro-aerobic) [50,51]	%	40.00	30.00	50.00		Triangular
Corn steep liquor price[12,24,44]	$/kg	0.06	0.05	0.07		Triangular
DAP price[12,24,44]	$/kg	0.97	0.69	1.10		Triangular
Limonene[52]						
Bioconversion time	*h*	*72.00*	*48.00*	*84.00*		*Uniform*
Glucose conversion	*wt%*	*16.21*	*6.05*	*32.41*		*Uniform*
Xylose conversion	*wt%*	*16.21*	*6.05*	*32.41*		*Uniform*
1,8-cineole[47,δ]						
Bioconversion time	*h*	*48*	*36*	*60*		*Uniform*
Glucose conversion	*wt%*	*18.3*	*10.52*	*36.69*		*Uniform*
Xylose conversion	*wt%*	*18.3*	*10.52*	*36.69*		*Uniform*
Linalool[47]						
Bioconversion time	*h*	*48*	*36*	*60*		*Uniform*
Glucose conversion	*wt%*	*18.3*	*5.05*	*36.69*		*Uniform*
Xylose conversion	*wt%*	*18.3*	*5.05*	*36.69*		*Uniform*
Bisabolene[52]						
Bioconversion time	*h*	*72.00*	*48.00*	*84.00*		*Uniform*
Glucose conversion	*wt%*	*16.21*	*11.5*	*32.41*		*Uniform*
Xylose conversion	*wt%*	*16.21*	*11.5*	*32.41*		*Uniform*
Epi-isozizaene[δ]						
Bioconversion time	*h*	*72.00*	*48.00*	*84.00*		*Uniform*
Glucose conversion	*wt%*	*7.18*	*6.05*	*32.41*		*Uniform*
Xylose conversion	*wt%*	*7.18*	*6.05*	*32.41*		*Uniform*
Recovery and separation						
Recovery of the jet fuel precursor (assumed[12])	wt%	97.00	95	99		Uniform
IL-recovery[20,22,23]	wt%	97.50	85.00	99.0		Triangular
Hydrogenation and oligomerization						
Hydrogen price[44]	$/kg	1.50	1.25	3.5		Triangular
Wastewater treatment						
Organic matter to biogas conversion[12]	wt%	86.00	85	91		Triangular
Lignin utilization						
Boiler chemicals price[12]	$/kg	5.00	4.00	6.00		Triangular
Natural gas price[b]	$/kg	0.22	0.10	0.44	0.10	Lognormal

[a]Estimated in this study considering chopped biomass transportation directly from the field to the biorefinery

[b]https://www.eia.gov/dnav/ng/hist/rngwhhdA.htm

[δ]Based on recent unpublished experimental results from JBEI/LBNL.

Table S3. Material and energy for feedstock supply system (after 5000 simulation runs)

Process	Materials	Units	Baseline value	Minimum	Maximum	Standard deviation
Nutrient & incentives	N	kg/t-DBS	7.35	2.03	22.39	4.18
	P	kg/t-DBS	1.45	0.12	9.92	1.54
	K	kg/t-DBS	10.19	0.99	54.62	7.28
Chopping (silage)	Diesel	L/t-DBS	3.09	1.10	9.36	1.29
Infield transportation	Diesel	L/t-DBS	0.38	0.21	0.77	0.09
Storage transport	Diesel	L/t-DBS	3.18	1.00	9.61	1.32
Storage at biorefinery	Tarp	m2/t-DBS	4.30	2.78	8.26	0.79
	Gravel	m2/t-DBS	3.51	2.27	6.74	0.65

Note: *'t' refers to metric ton, and 'DBS' refers to dry biomass sorghum at biorefinery gate*

Table S4. Material and energy for limonane via limonene (after 5000 simulation runs)

Life-cycle stages	Parameters	Unit	Baseline	Minimum	Maximum	Standard deviation
Feedstock supply logistics	Steam	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Acetate	kg/kg-Limonane via limonene	0.26	0.13	0.50	0.08
	Ash	kg/kg-Limonane via limonene	0.92	0.27	2.59	0.40
	Cellulose	kg/kg-Limonane via limonene	4.29	1.90	8.69	1.33
	Extractive	kg/kg-Limonane via limonene	1.25	0.00	4.54	0.94
	Hemicellulose	kg/kg-Limonane via limonene	2.74	1.25	5.31	0.85
	Lignin	kg/kg-Limonane via limonene	1.98	0.88	4.55	0.68
	Proteins	kg/kg-Limonane via limonene	0.53	0.26	1.00	0.16
	Moisture	kg/kg-Limonane via limonene	7.98	3.90	15.26	2.45
Feedstock handling	Steam	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Electricity	kWh/kg-Limonane via limonene	0.39	0.19	0.74	0.12
Pretreatment	Steam	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Steam 180°C	kg/kg-Limonane via limonene	1.04	0.51	2.01	0.32
	Electricity	kWh/kg-Limonane via limonene	0.10	0.05	0.21	0.03
	Ionic liquid	kg/kg-Limonane via limonene	0.12	0.03	0.95	0.19
	Sulfuric Acid	kg/kg-Limonane via limonene	0.93	0.45	1.61	0.28
	Water	kg/kg-Limonane via limonene	9.26	4.52	16.94	2.81
Hydrolysis and fermentation	Steam	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-Limonane via limonene	133.71	41.64	252.20	44.70
	Steam 180°C	kg/kg-Limonane via limonene	0.73	0.37	1.35	0.22
	Electricity	kWh/kg-Limonane via limonene	8.44	2.61	18.98	3.07
	Corn Liquor	kg/kg-Limonane via limonene	0.15	0.07	0.27	0.04
	Diammonium phosphate	kg/kg-Limonane via limonene	0.02	0.01	0.03	0.01
	Enzyme	kg/kg-Limonane via limonene	0.09	0.02	0.13	0.02
	Water	kg/kg-Limonane via limonene	16.64	8.38	31.12	5.04
	Air	kg/kg-Limonane via limonene	318.84	82.60	1214.28	172.04
	Inoculum	kg/kg-Limonane via limonene	0.03	0.02	0.06	0.01

Contd.

Table S4. Material and energy for limonane via limonene (after 5000 simulation runs- contd.)

Recovery and separation	Steam	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-Limonane via limonene	1630.70	812.25	2993.97	488.62
	Steam 226°C	kg/kg-Limonane via limonene	23.99	11.95	43.95	7.19
	Steam 180°C	kg/kg-Limonane via limonene	10.12	5.01	18.58	3.05
	Electricity	kWh/kg-Limonane via limonene	0.14	0.07	0.26	0.04
Hydrogenation	Steam	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-Limonane via limonene	20.07	20.07	20.08	0.00
	Chilled Water	kg/kg-Limonane via limonene	3.67	3.67	3.67	0.00
	Steam330°C	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Electricity	kWh/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Hydrogen	kg/kg-Limonane via limonene	0.01	0.01	0.01	0.00
	Pd/AC catalyst	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
Wastewater treatment	Steam	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Steam 180°C	kg/kg-Limonane via limonene	0.81	0.41	1.50	0.24
	Electricity	kWh/kg-Limonane via limonene	0.43	0.21	0.80	0.13
	Water	kg/kg-Limonane via limonene	37.93	18.51	72.51	11.66
	Air	kg/kg-Limonane via limonene	34.30	16.74	65.57	10.54
	CIP	kg/kg-Limonane via limonene	0.06	0.03	0.12	0.02
	WWT nutrients	kg/kg-Limonane via limonene	0.01	0.00	0.02	0.00
Lignin utilization	Steam	kg/kg-Limonane via limonene	0.00	0.00	0.00	0.00
	Cooling water	kg/kg-Limonane via limonene	1445.18	662.51	2774.59	457.74
	Electricity	kWh/kg-Limonane via limonene	0.70	0.32	1.34	0.22
	Methane	kg/kg-Limonane via limonene	1.39	0.68	2.66	0.43
	Water	kg/kg-Limonane via limonene	112.47	54.89	215.02	34.57
	Air	kg/kg-Limonane via limonene	419.87	204.92	802.68	129.04

Table S5. Material and energy for limonane via 1,8 cineole (after 5000 simulation runs)

Life-cycle stages	Parameters	Unit	Baseline	Minimum	Maximum	Standard deviation
Feedstock supply logistics	Steam	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Acetate	kg/kg-limonane via 1,8 cineole	0.25	0.14	0.47	0.07
	Ash	kg/kg-limonane via 1,8 cineole	0.87	0.28	1.95	0.37
	Cellulose	kg/kg-limonane via 1,8 cineole	4.06	2.04	7.58	1.18
	Extractive	kg/kg-limonane via 1,8 cineole	1.19	0.00	4.35	0.96
	Hemicellulose	kg/kg-limonane via 1,8 cineole	2.60	1.32	4.77	0.75
	Lignin	kg/kg-limonane via 1,8 cineole	1.87	0.93	4.46	0.67
	Proteins	kg/kg-limonane via 1,8 cineole	0.50	0.27	0.94	0.15
	Moisture	kg/kg-limonane via 1,8 cineole	7.56	4.13	14.32	2.23
Feedstock handling	Steam	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Electricity	kWh/kg-limonane via 1,8 cineole	0.37	0.20	0.69	0.11
Pretreatment	Steam	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Steam 226°C	kg/kg-limonane via 1,8 cineole	0.92	0.50	1.80	0.28
	Electricity	kWh/kg-limonane via 1,8 cineole	0.10	0.06	0.19	0.03
	Ionic liquid	kg/kg-limonane via 1,8 cineole	0.11	0.03	0.91	0.19
	Sulfuric Acid	kg/kg-limonane via 1,8 cineole	0.88	0.49	1.55	0.26
	Water	kg/kg-limonane via 1,8 cineole	8.74	4.81	16.21	2.54
Hydrolysis and fermentation	Steam	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-limonane via 1,8 cineole	221.37	123.90	454.95	90.38
	Steam 180°C	kg/kg-limonane via 1,8 cineole	0.69	0.40	1.29	0.20
	Electricity	kWh/kg-limonane via 1,8 cineole	5.59	3.10	13.13	2.73
	Corn Liquor	kg/kg-limonane via 1,8 cineole	0.14	0.08	0.26	0.04
	Diammonium phosphate	kg/kg-limonane via 1,8 cineole	0.02	0.01	0.03	0.01
	Enzyme	kg/kg-limonane via 1,8 cineole	0.08	0.02	0.13	0.02
	Water	kg/kg-limonane via 1,8 cineole	15.81	9.20	29.78	4.58
	Air	kg/kg-limonane via 1,8 cineole	201.45	101.32	819.45	147.42
	Inoculum	kg/kg-limonane via 1,8 cineole	0.03	0.02	0.06	0.01
Recovery and separation	Steam	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-limonane via 1,8 cineole	1528.85	849.21	2812.55	437.28
	Steam 226°C	kg/kg-limonane via 1,8 cineole	0.01	0.01	0.01	0.00
	Steam 180°C	kg/kg-limonane via 1,8 cineole	9.59	5.31	17.65	2.75
	Steam330°C	kg/kg-limonane via 1,8 cineole	20.69	11.47	38.25	5.93
	Electricity	kWh/kg-limonane via 1,8 cineole	0.13	0.07	0.25	0.04

Contd.

Table S5. Material and energy for limonane via 1,8 cineole (after 5000 simulation runs-contd.)

Hydrogenation	Steam	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-limonane via 1,8 cineole	4.05	3.88	4.32	0.10
	Chilled Water	kg/kg-limonane via 1,8 cineole	22.73	22.73	22.73	0.00
	Cooling water	kg/kg-limonane via 1,8 cineole	0.62	0.62	0.62	0.00
	Steam 180°C	kg/kg-limonane via 1,8 cineole	0.15	0.15	0.15	0.00
	Electricity	kWh/kg-limonane via 1,8 cineole	0.01	0.01	0.01	0.00
	Cyclohexane	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Hydrogen	kg/kg-limonane via 1,8 cineole	0.02	0.02	0.02	0.00
	Pd/AC catalyst	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Trifluoroacetic acid	kg/kg-limonane via 1,8 cineole	0.03	0.03	0.03	0.00
Wastewater treatment	Steam	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Steam 180°C	kg/kg-limonane via 1,8 cineole	0.77	0.43	1.38	0.22
	Electricity	kWh/kg-limonane via 1,8 cineole	0.41	0.23	0.76	0.12
	Water	kg/kg-limonane via 1,8 cineole	35.95	19.63	68.05	10.58
	Air	kg/kg-limonane via 1,8 cineole	32.50	17.75	61.53	9.57
	WWT nutrients	kg/kg-limonane via 1,8 cineole	0.01	0.00	0.01	0.00
Lignin utilization	Steam	kg/kg-limonane via 1,8 cineole	0.00	0.00	0.00	0.00
	Cooling water	kg/kg-limonane via 1,8 cineole	1251.60	635.56	2422.52	392.19
	Electricity	kWh/kg-limonane via 1,8 cineole	2.15	1.10	4.16	0.67
	Methane	kg/kg-limonane via 1,8 cineole	1.05	0.57	1.99	0.31
	Water	kg/kg-limonane via 1,8 cineole	96.23	52.54	182.18	28.33
	Air	kg/kg-limonane via 1,8 cineole	397.92	217.26	753.31	117.14

Table S6. Material and energy for RJ-4 (after 5000 simulation runs)

Life-cycle stages	Parameters	Unit	Baseline	Minimum	Maximum	Standard deviation
Feedstock supply logistics	Steam	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	Acetate	kg/kg-RJ-4	0.26	0.13	0.62	0.10
	Ash	kg/kg-RJ-4	0.91	0.28	3.18	0.46
	Cellulose	kg/kg-RJ-4	4.25	1.89	10.64	1.61
	Extractive	kg/kg-RJ-4	1.24	0.00	5.17	1.02
	Hemicellulose	kg/kg-RJ-4	2.72	1.25	6.51	1.02
	Lignin	kg/kg-RJ-4	1.96	0.88	5.16	0.80
	Proteins	kg/kg-RJ-4	0.52	0.26	1.23	0.20
	Moisture	kg/kg-RJ-4	7.91	3.90	18.69	2.98
Feedstock handling	Steam	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	Electricity	kWh/kg-RJ-4	0.38	0.19	0.91	0.14
Pretreatment	Steam	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	Steam 226°C	kg/kg-RJ-4	0.96	0.47	2.19	0.37
	Electricity	kWh/kg-RJ-4	0.10	0.05	0.26	0.04
	Ionic liquid	kg/kg-RJ-4	0.12	0.03	1.08	0.21
	Sulfuric acid	kg/kg-RJ-4	0.92	0.45	1.96	0.34
	Water	kg/kg-RJ-4	9.11	4.48	20.70	3.41
Hydrolysis and fermentation	Steam	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-RJ-4	231.68	82.31	559.24	92.12
	Steam 180°C	kg/kg-RJ-4	0.73	0.38	1.60	0.26
	Electricity	kWh/kg-RJ-4	5.85	2.03	17.12	2.61
	Corn Liquor	kg/kg-RJ-4	0.15	0.07	0.34	0.05
	Diammonium phosphate	kg/kg-RJ-4	0.02	0.01	0.04	0.01
	Enzyme	kg/kg-RJ-4	0.09	0.02	0.15	0.03
	Water	kg/kg-RJ-4	16.55	8.52	36.95	6.10
	Air	kg/kg-RJ-4	210.59	61.16	1064.53	143.98
	Inoculum	kg/kg-RJ-4	0.03	0.02	0.08	0.01
Recovery and separation	Steam	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-RJ-4	1598.29	801.79	3631.86	587.16
	Steam 226°C	kg/kg-RJ-4	0.01	0.01	0.02	0.00
	Steam 180°C	kg/kg-RJ-4	10.02	5.01	22.77	3.69
	Steam330°C	kg/kg-RJ-4	21.63	10.84	49.05	7.95
	Electricity	kWh/kg-RJ-4	0.14	0.07	0.31	0.05

Contd.

Table S6. Material and energy for RJ-4 (after 5000 simulation runs-contd.)

Hydrogenation	Steam	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-RJ-4	4.62	4.62	4.62	0.00
	Chilled Water	kg/kg-RJ-4	30.82	30.82	30.82	0.00
	Steam 226°C	kg/kg-RJ-4	0.02	0.02	0.02	0.00
	Steam330°C	kg/kg-RJ-4	0.21	0.21	0.21	0.00
	Electricity	kWh/kg-RJ-4	0.00	0.00	0.00	0.00
	AlCl3	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	dehydrating Cat	kg/kg-RJ-4	0.06	0.06	0.06	0.00
	Hydrogen	kg/kg-RJ-4	0.01	0.01	0.01	0.00
	Pd/AC Catalyst	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	Grubbs' catalysts (Ru)	kg/kg-RJ-4	0.00	0.00	0.00	0.00
Wastewater treatment	Steam	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	Steam 226°C	kg/kg-RJ-4	0.75	0.38	1.71	0.27
	Electricity	kWh/kg-RJ-4	0.43	0.21	0.98	0.16
	Water	kg/kg-RJ-4	37.58	18.52	88.84	14.14
	Air	kg/kg-RJ-4	33.98	16.74	80.33	12.78
	WWT nutrients	kg/kg-RJ-4	0.01	0.00	0.02	0.00
Lignin utilization	Steam	kg/kg-RJ-4	0.00	0.00	0.00	0.00
	Cooling water	kg/kg-RJ-4	1240.72	577.07	2736.12	476.50
	Electricity	kWh/kg-RJ-4	2.16	1.01	4.75	0.83
	Methane	kg/kg-RJ-4	0.94	0.46	2.23	0.35
	Water	kg/kg-RJ-4	90.87	47.06	227.07	36.15
	Air	kg/kg-RJ-4	415.97	204.99	983.44	156.51

Table S7. Material and energy for Bisabolane (after 5000 simulation runs)

Life-cycle stages	Parameters	Unit	Baseline	Minimum	Maximum	Standard deviation
Feedstock supply logistics	Steam	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
	Acetate	kg/kg-Bisabolane	0.26	0.13	0.34	0.04
	Ash	kg/kg-Bisabolane	0.92	0.24	1.71	0.29
	Cellulose	kg/kg-Bisabolane	4.27	1.83	5.27	0.72
	Extractive	kg/kg-Bisabolane	1.25	0.00	3.08	0.75
	Hemicellulose	kg/kg-Bisabolane	2.74	1.20	3.38	0.47
	Lignin	kg/kg-Bisabolane	1.97	0.86	3.10	0.41
	Proteins	kg/kg-Bisabolane	0.52	0.25	0.67	0.09
	Moisture	kg/kg-Bisabolane	7.96	3.82	10.15	1.35
Feedstock handling	Steam	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
	Electricity	kWh/kg-Bisabolane	0.39	0.19	0.49	0.07
Pretreatment	Steam	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
	Steam 180°C	kg/kg-Bisabolane	1.04	0.50	1.37	0.18
	Electricity	kWh/kg-Bisabolane	0.10	0.05	0.13	0.02
	Ionic liquid	kg/kg-Bisabolane	0.12	0.02	0.65	0.16
	Sulfuric Acid	kg/kg-Bisabolane	0.93	0.43	1.13	0.16
	Water	kg/kg-Bisabolane	9.24	4.43	11.49	1.55
Hydrolysis and fermentation	Steam	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-Bisabolane	296.27	87.89	354.06	67.09
	Steam 226°C	kg/kg-Bisabolane	0.68	0.33	0.85	0.11
	Electricity	kWh/kg-Bisabolane	8.41	2.47	11.32	2.10
	Corn Liquor	kg/kg-Bisabolane	0.15	0.07	0.18	0.03
	Diammonium phosphate	kg/kg-Bisabolane	0.02	0.01	0.02	0.00
	Enzyme	kg/kg-Bisabolane	0.09	0.02	0.09	0.01
	Water	kg/kg-Bisabolane	16.58	7.96	21.11	2.81
	Air	kg/kg-Bisabolane	317.89	80.73	720.51	114.11
	Inoculum	kg/kg-Bisabolane	0.03	0.02	0.04	0.01
Recovery and separation	Steam	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-Bisabolane	1623.43	788.64	2013.42	269.63
	Steam330°C	kg/kg-Bisabolane	22.05	10.64	27.69	3.71
	Steam 180°C	kg/kg-Bisabolane	10.09	4.86	12.51	1.69
	Steam 226°C	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
	Electricity	kWh/kg-Bisabolane	0.14	0.07	0.17	0.02

Contd.

Table S7. Material and energy for Bisabolane (after 5000 simulation runs-contd.)

Hydrogenation	Steam	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-Bisabolane	22.14	22.14	22.14	0.00
	Chilled Water	kg/kg-Bisabolane	22.19	22.19	22.19	0.00
	Steam330°C	kg/kg-Bisabolane	0.14	0.14	0.14	0.00
	Electricity	kWh/kg-Bisabolane	0.00	0.00	0.00	0.00
	Hydrogen	kg/kg-Bisabolane	0.02	0.02	0.02	0.00
	Pd/AC Catalyst	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
Wastewater treatment	Steam	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
	Steam 226°C	kg/kg-Bisabolane	0.75	0.37	0.92	0.12
	Electricity	kWh/kg-Bisabolane	0.43	0.21	0.54	0.07
	Water	kg/kg-Bisabolane	37.82	18.14	48.24	6.41
	Air	kg/kg-Bisabolane	34.19	16.41	43.62	5.80
	WWT nutrients	kg/kg-Bisabolane	0.01	0.00	0.01	0.00
Lignin utilization	Steam	kg/kg-Bisabolane	0.00	0.00	0.00	0.00
	Cooling water	kg/kg-Bisabolane	1575.88	713.30	2007.97	283.48
	Electricity	kWh/kg-Bisabolane	2.04	0.93	2.61	0.37
	Methane	kg/kg-Bisabolane	1.66	0.80	2.11	0.28
	Water	kg/kg-Bisabolane	107.16	53.73	142.87	19.08
	Air	kg/kg-Bisabolane	418.61	200.85	534.05	71.00

Table S8. Material and energy for Epi-isozizaane (after 5000 simulation runs)

Life-cycle stages	Parameters	Unit	Baseline	Minimum	Maximum	Standard deviation
Feedstock supply logistics	Steam	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Acetate	kg/kg-Epi-isozizaane	0.26	0.13	0.45	0.07
	Ash	kg/kg-Epi-isozizaane	0.92	0.26	2.27	0.37
	Cellulose	kg/kg-Epi-isozizaane	4.27	1.88	7.60	1.15
	Extractive	kg/kg-Epi-isozizaane	1.25	0.00	4.13	0.89
	Hemicellulose	kg/kg-Epi-isozizaane	2.74	1.23	4.65	0.74
	Lignin	kg/kg-Epi-isozizaane	1.97	0.87	4.14	0.61
	Proteins	kg/kg-Epi-isozizaane	0.52	0.25	0.90	0.14
	Moisture	kg/kg-Epi-isozizaane	0.12	3.87	13.61	2.13
Feedstock handling	Steam	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Electricity	kWh/kg-Epi-isozizaane	0.39	0.19	0.66	0.10
Pretreatment	Steam	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Steam 180°C	kg/kg-Epi-isozizaane	1.04	0.51	1.83	0.28
	Electricity	kWh/kg-Epi-isozizaane	0.10	0.05	0.18	0.03
	Ionic liquid	kg/kg-Epi-isozizaane	0.12	0.03	0.86	0.18
	Sulfuric Acid	kg/kg-Epi-isozizaane	0.93	0.45	1.47	0.25
	Water	kg/kg-Epi-isozizaane	9.24	4.50	15.41	2.45
Hydrolysis and fermentation	Steam	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-Epi-isozizaane	296.31	91.32	490.72	89.74
	Steam 226°C	kg/kg-Epi-isozizaane	0.68	0.34	1.14	0.18
	Electricity	kWh/kg-Epi-isozizaane	8.41	2.57	16.61	2.78
	Corn Liquor	kg/kg-Epi-isozizaane	0.15	0.07	0.25	0.04
	Diammonium phosphate	kg/kg-Epi-isozizaane	0.02	0.01	0.03	0.01
	Enzyme	kg/kg-Epi-isozizaane	0.09	0.02	0.12	0.02
	Water	kg/kg-Epi-isozizaane	16.58	8.26	28.30	4.40
	Air	kg/kg-Epi-isozizaane	317.94	82.07	1062.00	154.61
	Inoculum	kg/kg-Epi-isozizaane	0.03	0.02	0.06	0.01
Recovery and separation	Steam	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-Epi-isozizaane	1623.66	805.55	2695.70	424.81
	Steam 180°C	kg/kg-Epi-isozizaane	10.09	4.97	16.77	2.65
	Steam 226°C	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Steam330°C	kg/kg-Epi-isozizaane	22.05	10.90	37.05	5.80
	Electricity	kWh/kg-Epi-isozizaane	0.14	0.07	0.23	0.04

Contd.

Table S8. Material and energy for Epi-isozizaane (after 5000 simulation runs-contd.)

Hydrogenation	Steam	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Cooling Water	kg/kg-Epi-isozizaane	22.14	22.14	22.14	0.00
	Chilled Water	kg/kg-Epi-isozizaane	22.19	22.18	22.19	0.00
	Steam330°C	kg/kg-Epi-isozizaane	0.14	0.14	0.14	0.00
	Electricity	kWh/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Hydrogen	kg/kg-Epi-isozizaane	0.02	0.02	0.02	0.00
	Pd/AC Catalyst	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
Wastewater treatment	Steam	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Steam 226°C	kg/kg-Epi-isozizaane	0.75	0.38	1.23	0.20
	Electricity	kWh/kg-Epi-isozizaane	0.43	0.21	0.72	0.11
	Water	kg/kg-Epi-isozizaane	37.82	18.39	64.67	10.14
	Air	kg/kg-Epi-isozizaane	34.20	16.63	58.48	9.17
	WWT nutrients	kg/kg-Epi-isozizaane	0.01	0.00	0.01	0.00
Lignin utilization	Steam	kg/kg-Epi-isozizaane	0.00	0.00	0.00	0.00
	Cooling water	kg/kg-Epi-isozizaane	1576.07	722.58	2770.38	437.74
	Electricity	kWh/kg-Epi-isozizaane	2.04	0.94	3.58	0.57
	Methane	kg/kg-Epi-isozizaane	1.66	0.81	2.84	0.44
	Water	kg/kg-Epi-isozizaane	107.18	54.52	191.74	30.15
	Air	kg/kg-Epi-isozizaane	418.67	203.55	715.92	112.28

S2. Selection of the type of probability distribution

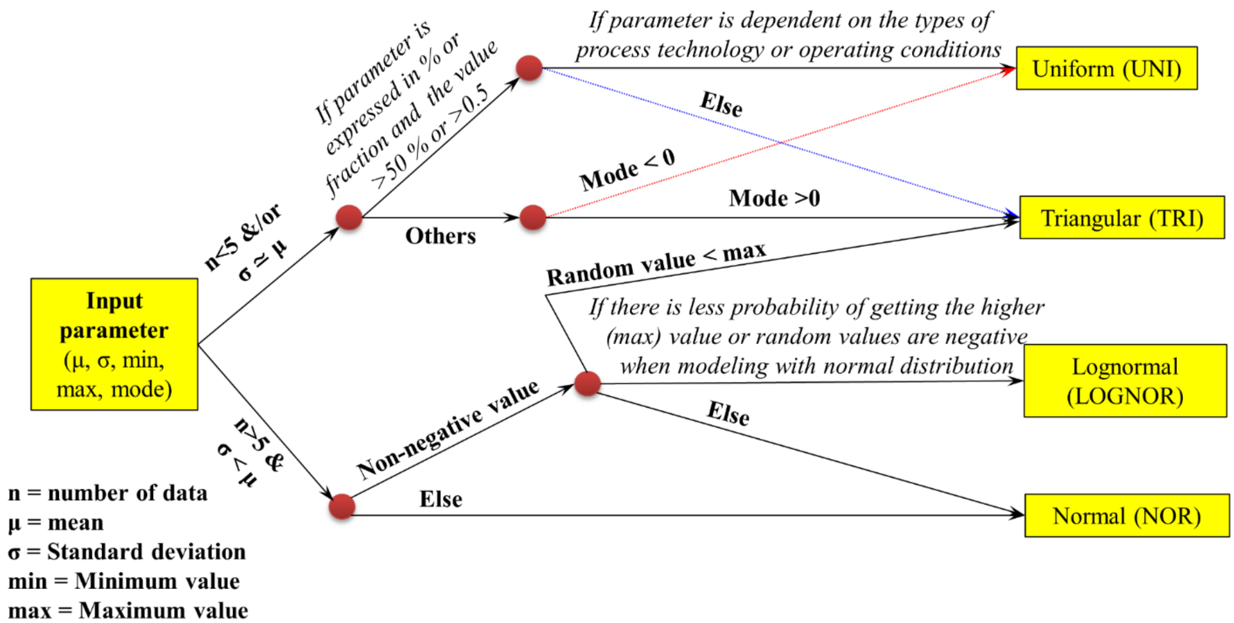


Figure S1. Selection criteria for different probability distributions considered in this study

S3. Fuel cost savings over flight ranges

The Breguet range equation illustrated in previous studies,[35,36] and the energy density of conventional and the selected renewable jet fuels (Table S1) are used to determine the fuel consumption over the flying range. We consider the lower heating values of fuels (Table S1). The Breguet range equation provides fuel consumption per passenger per 100 km flight distance over the flown distance. The inputs to the Breguet range equation can be obtained from a payload range diagram of an aircraft. The payload range diagram provides the maximum possible take-off mass based on the planned flight distance. The previous study[36] has illustrated the detailed methods. While the higher energy density provides fuel consumption benefits, it also increases the take-off weights of an aircraft, if fully loaded. Our model accounts for these variations. We consider Boeing 777-300ER, as an example, and determine fuel cost and GHG emissions over the range. The fuel cost is determined considering the fuel consumption over the range obtained from the Breguet range equation and an equal fuel price of $1.68/L for both conventional and renewable jet fuels. This is the projected price of conventional jet fuel in 2050,[37] which is in 2018 dollars. Based on the results of this study, we assume that the selected renewable jet fuel molecules could be produced at the same price in 2050, which require future research and development efforts. Further, we illustrate the total fuel cost savings considering a typical domestic flight (San Francisco (SFO), USA to New York (JFK), USA- 2247 nm or 4162 km) and an international flight (from San Francisco (SFO), USA to London (LHR), UK- 4664 nm or 8638 km).[35,36] These are determined by estimating the fuel saving for the entire flight based on a fuel price of $1.68/L.

S4. Capital investment and operating cost

The required capital and operating costs to produce different jet fuel molecules from biomass sorghum feedstock of 1814 metric ton (t)/day (2000 dry ton/day) is shown in Figure S2. The selected jet fuel molecules, including limonane, bisabolane, and epi-isozizaane, require the similar level of total capital investment of $12/L ($47/gal). This capital investment is 6.7 times greater than the capital investment of a typical cellulosic ethanol production facility.[12] The main reasons for this increased capital investment are 4.1 times lower total end-product yield with the similar feedstock quantity and structural compositions, as well as capital-intensive IL recovery (pervaporation[53]) and jet fuel precursor recovery methods. The capital investment can be reduced by building a larger-scale biorefinery (utilizing the large quantity of biomass feedstock), by increasing annual operating hours (reduces the required size of process equipment), and by increasing the yield and productivity (titer) of jet fuel precursors. For instance, when the biorefinery capacity was increased from the baseline capacity of 60 million liters/year (15.8 million gallons/year) to 189 million liters/year (50 million gallons/year) by utilizing dry biomass sorghum of 2721.5 t/day (3000 tons/day) with optimal process parameters (discussed in the *Optimal jet fuel selling price* section), the capital investment decreased to $3.9/L ($15/gal). However, increasing feedstock intake is also likely to increase biomass transportation and logistics costs. Other jet fuel molecules (limonane via 1,8-cineole and RJ-4) require additional equipment for hydrogenation and/or oligomerization processes, but require 12% less capital investment overall. This is mainly due to 13% lower retention time (higher productivity) during bioconversion to their precursors compared to other jet fuel molecules. Generally, the direct fixed capital accounts for 59% of the total capital investment followed by 36% for indirect cost, 4.7% for working capital, and land accounts for the remaining fraction. The lignin utilization and recovery sections are the major contributors to the direct capital investment collectively responsible for 67% of the total direct fixed capital cost. Engineering pervaporation systems with cheap materials/improved designs would reduce those capital costs. Alternatively, a cheap IL (price close to sulfuric acid or ammonia) could eliminate the IL-recovery process altogether, resulting in significantly lower capital investments.

For operating costs, process chemicals, specifically enzymes and IL, are the major contributors, collectively responsible for 43% of the total operating cost followed by 33% for biomass feedstock, 8% for facility dependent, 7% for utilities, and 5% for labor. The facility-dependent cost comprises operation and maintenance cost, property tax, and insurance. The variation in operating costs among the jet fuel molecules is mainly due to different process chemicals and catalysts required for the hydrogenation and/or oligomerization process. In contrast to other jet fuel molecules, RJ-4 requires additional catalytic conversion and oligomerization processes requiring additional metal catalysts[54] such as Ru (metathesis catalyst) and $AlCl_3$ (isomerizing catalyst) resulting in 23% higher operating costs.

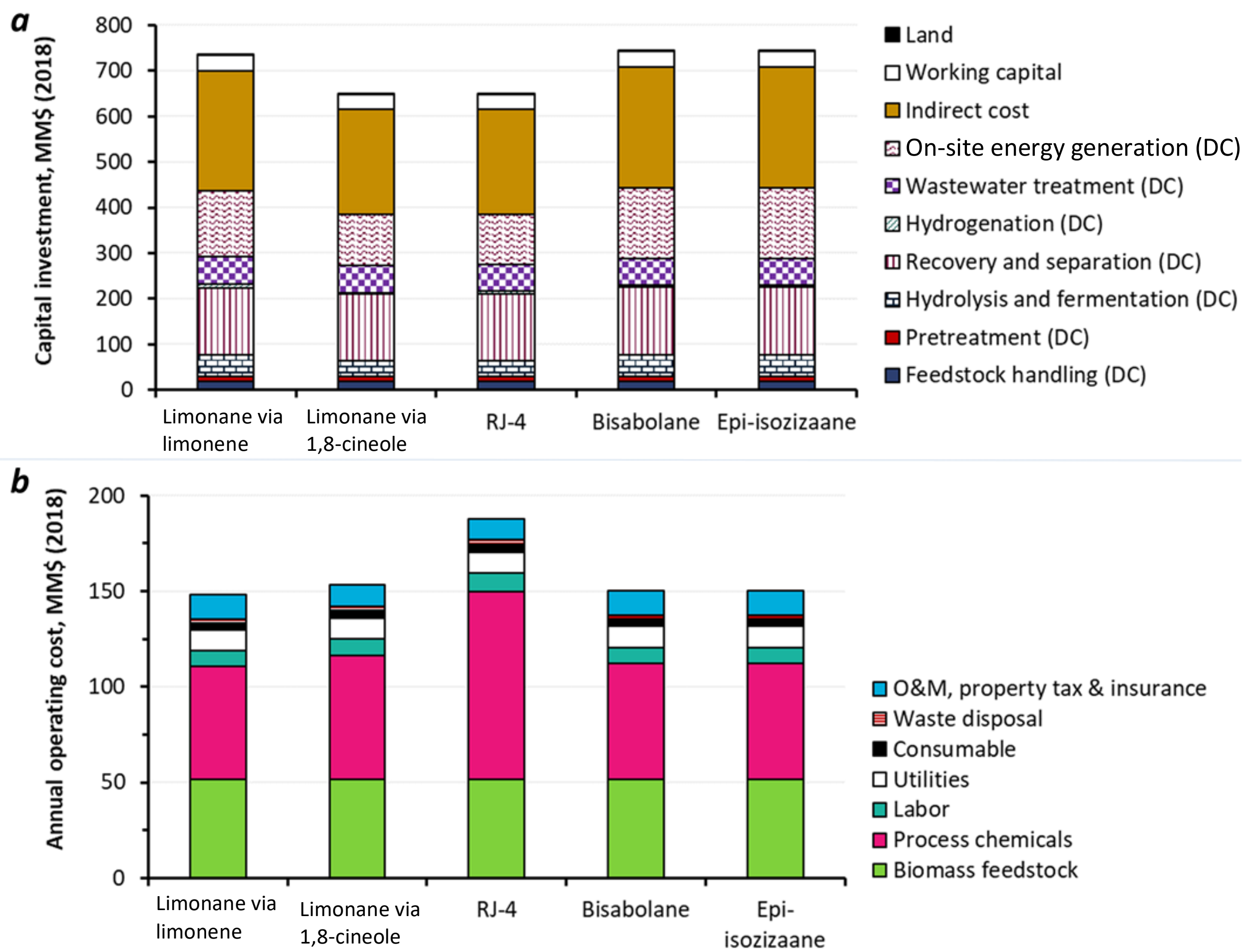


Figure S2. Capital investment (a) and annual operating cost (b) of different jet fuel molecules. 'DC' refers to direct cost; 'O&M' refer to operations and maintenance costs. These results correspond to the baseline scenario, i.e., using average value of input parameters.

S5. Minimum selling price with different pathways and product yields

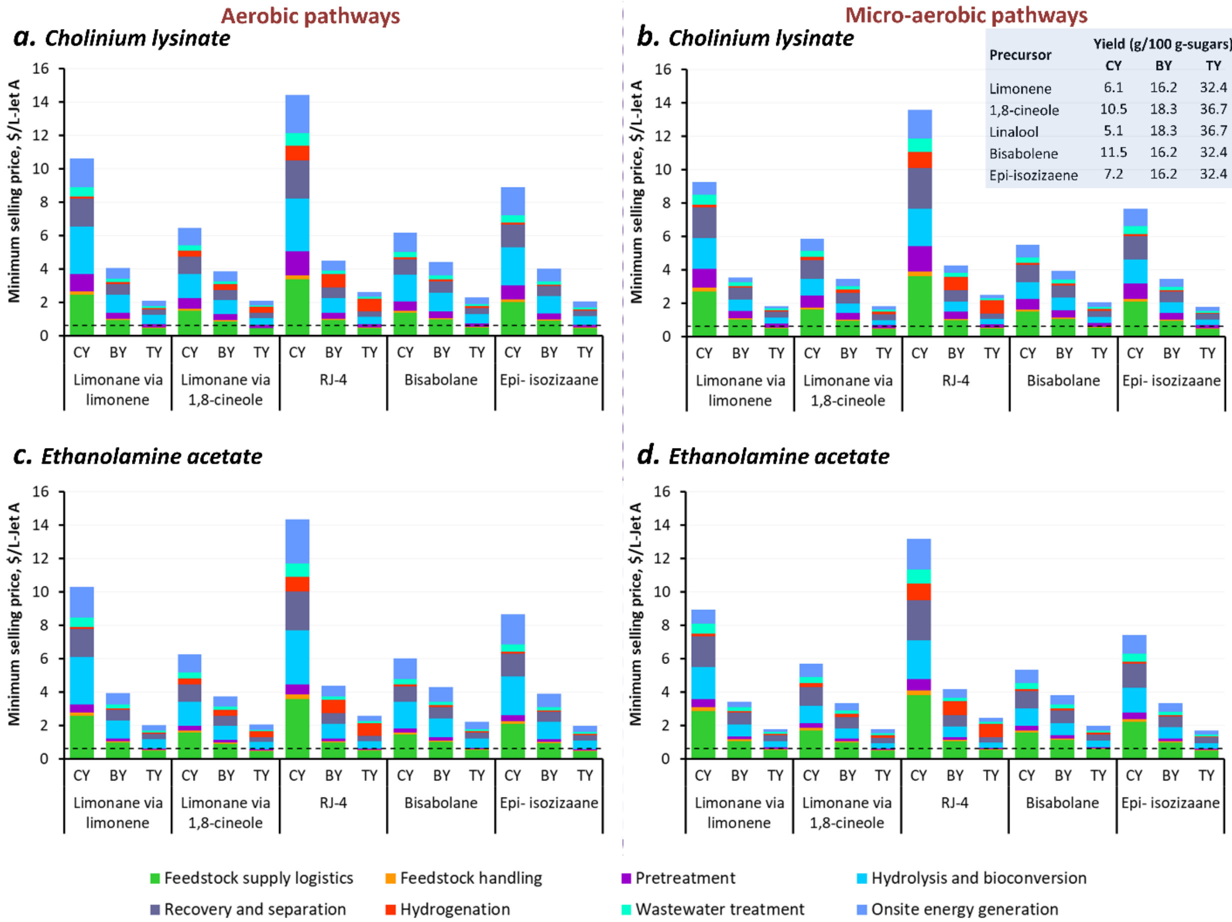
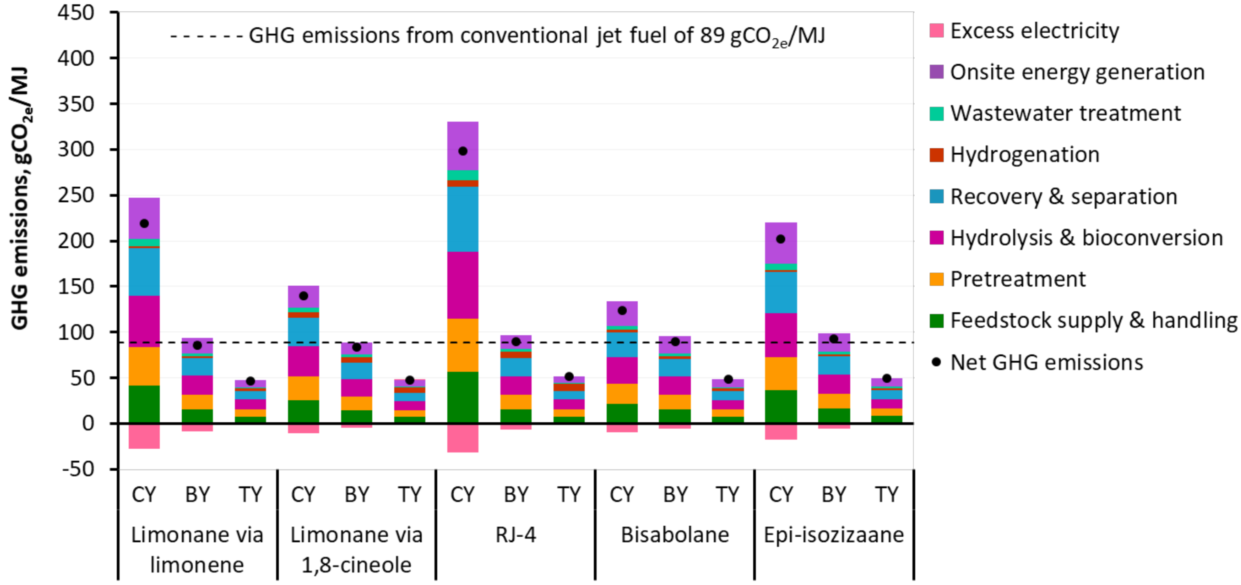


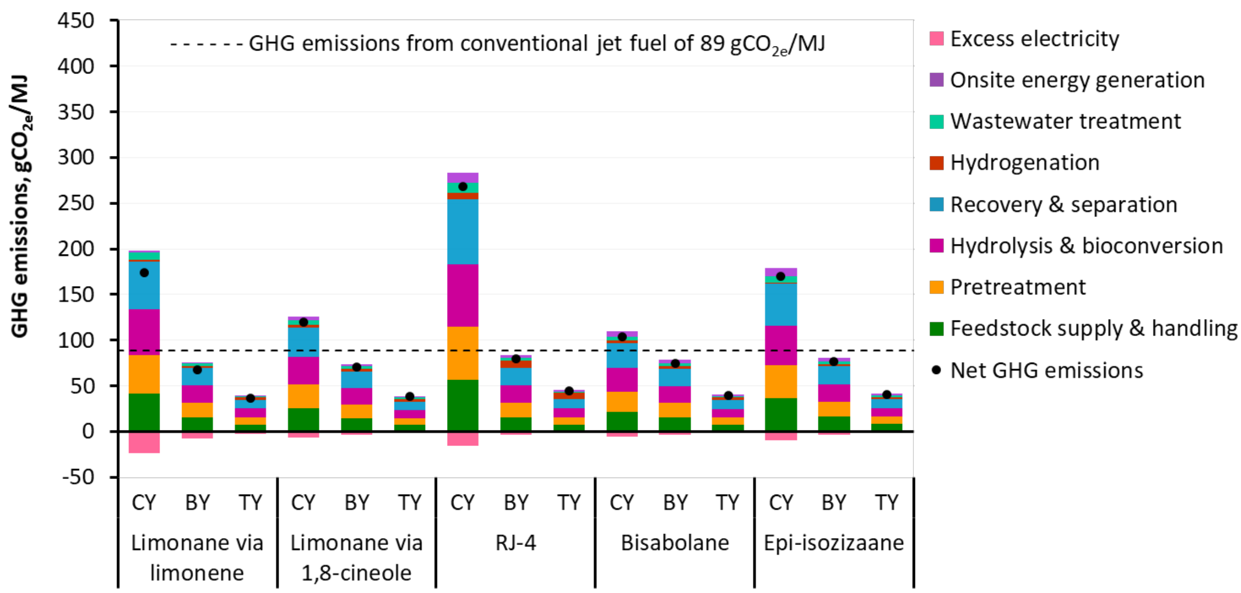
Figure S3. Minimum selling price of renewable jet fuel blendstocks under different bioconversion pathways and product yields. In this Figure, 'CY', 'BY', and 'TY' refer to current, baseline, and maximum theoretical yields, respectively. For comparison, the horizontal dashed line (- - - - - -) refers to the 10-year average Jet fuel retail price ($/L) of 0.61.[55]

S6. Greenhouse gas emissions associated with different jet fuel molecules under different bioconversion pathways

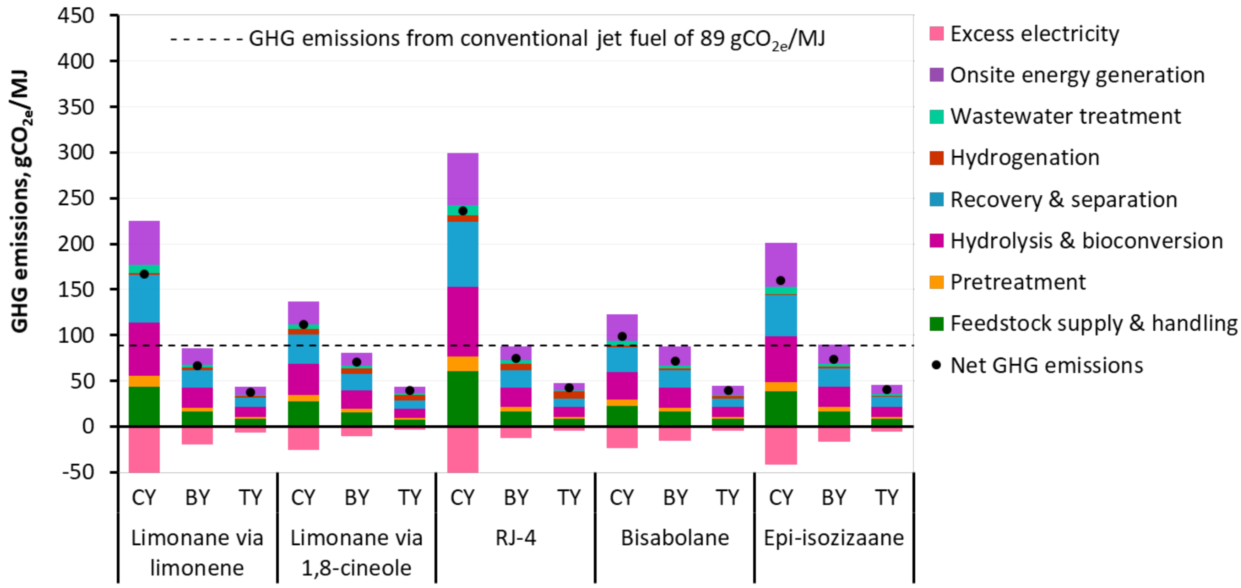
a. [Ch][Lys] based pretreatment and aerobic bioconversion



b. [Ch][Lys] based pretreatment and micro-aerobic bioconversion



c. [EOA][OAc] based pretreatment and aerobic bioconversion



d. [EOA][OAc] based pretreatment and micro-aerobic bioconversion

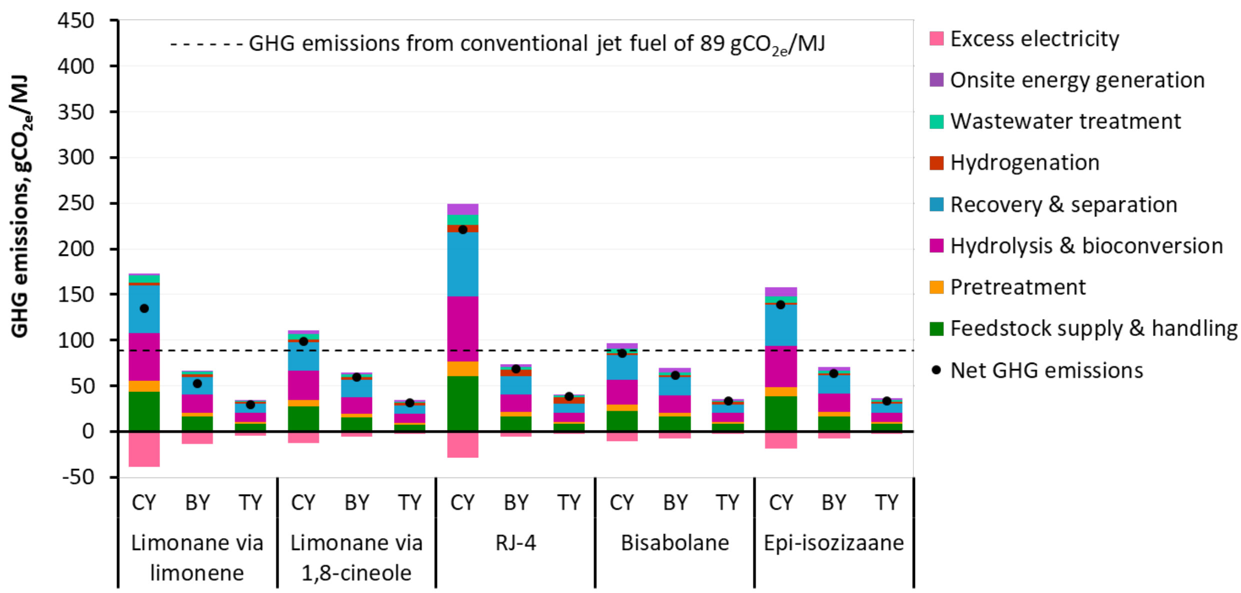
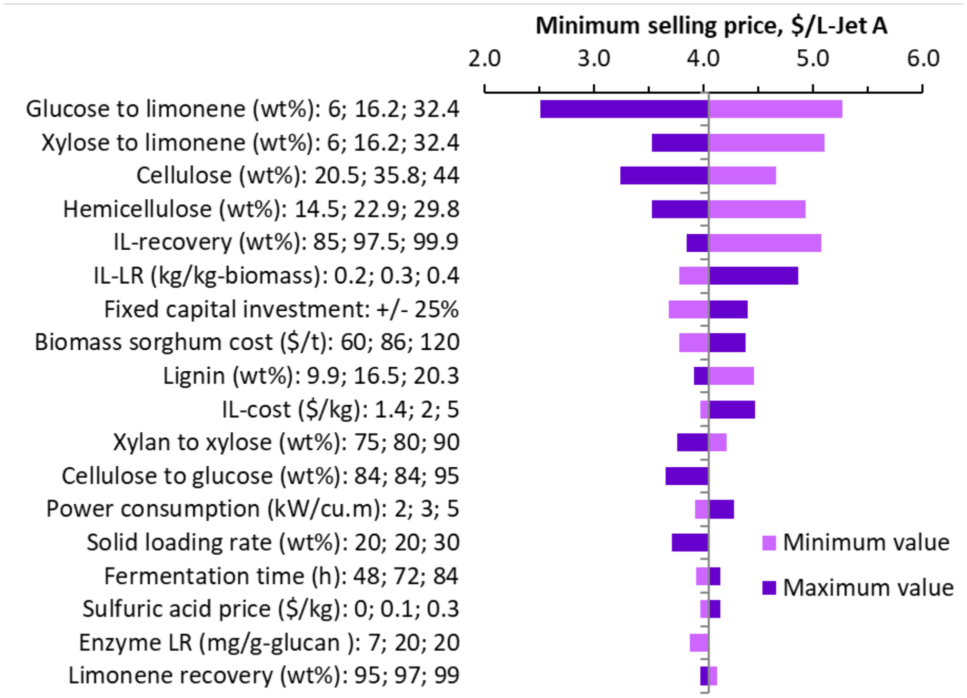


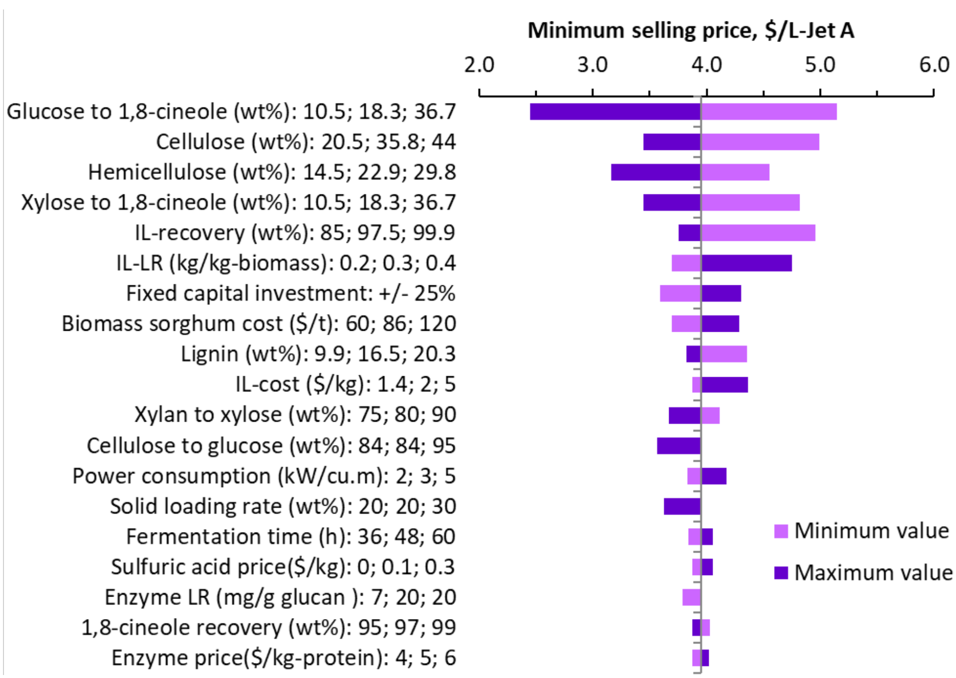
Figure S4. GHG emissions of different jet fuel molecules under different bioconversion pathways and yield scenarios. Current yield (CY) refers to the baseline values with current best-reported product yield; Baseline Yield (BY) refers to the baseline values with 50% of stoichiometric theoretical yield; and Theoretical yield (TY) refers to the baseline values with 100% of stoichiometric theoretical yield.

S7. Sensitivity analysis

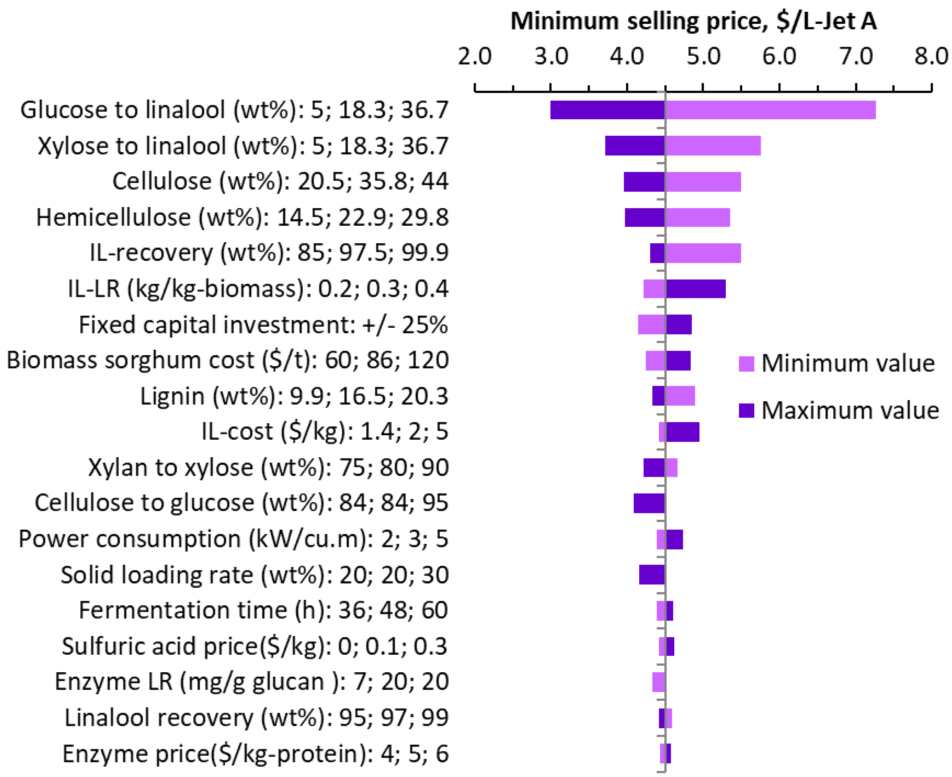
a. Limonane via limonene



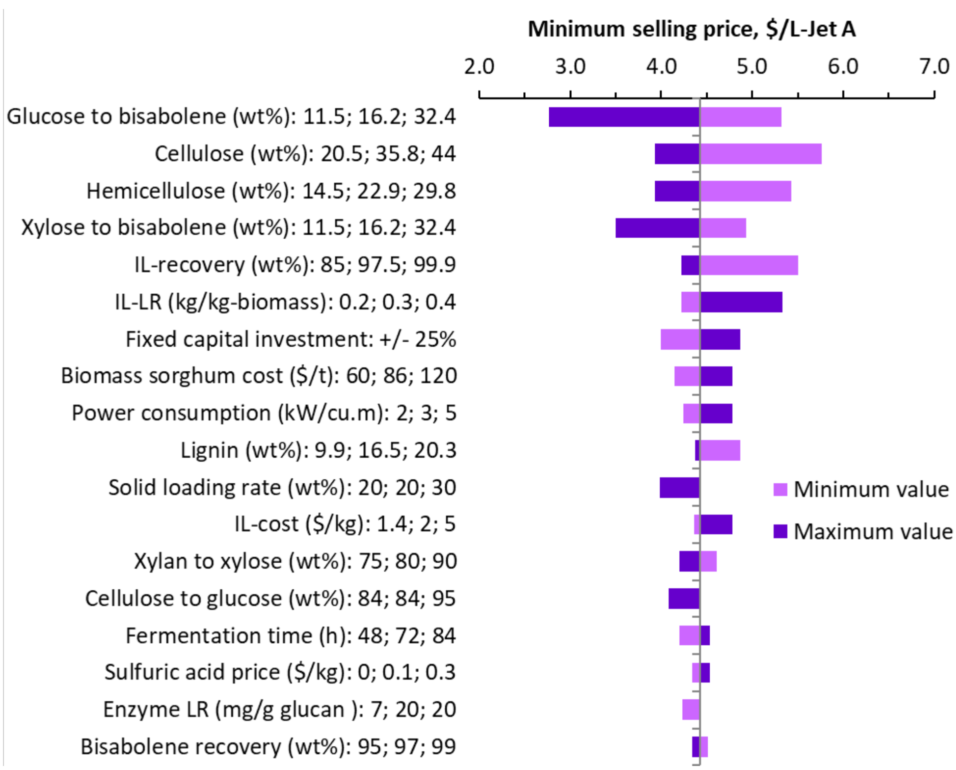
b. Limonane via 1,8-cineole



c. RJ-4



d. Bisabolane



e. Epi-isozizaane

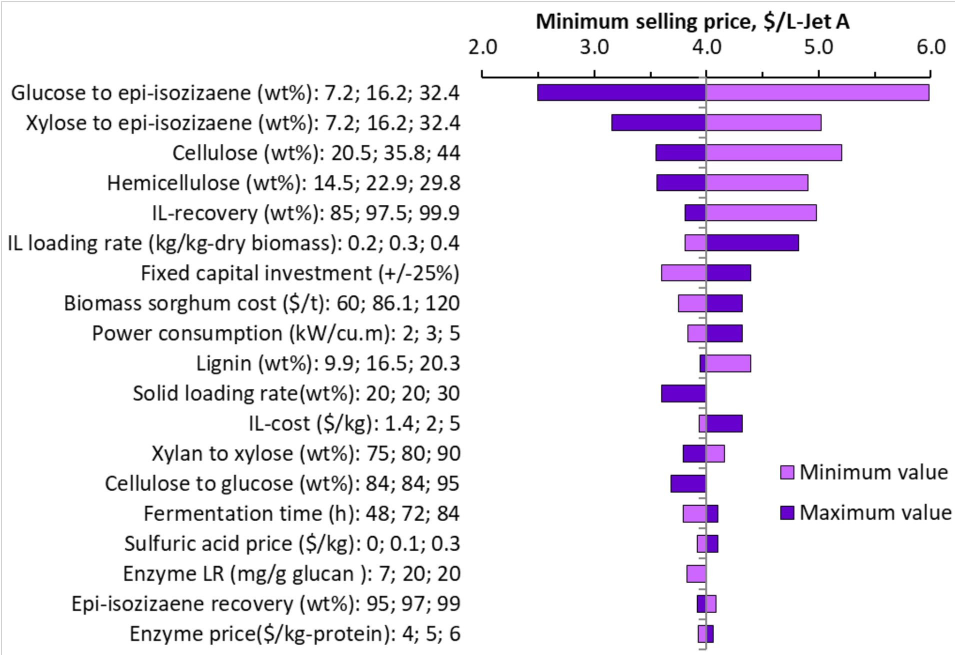


Figure S5. Most influential input parameters to the jet fuel selling price. ‘LR’ and ‘IL’ refer to loading rate and ionic liquid, respectively.

S8. Uncertainties associated with the different stages of Jet fuel production system

S8.1 Feedstock supply and handling

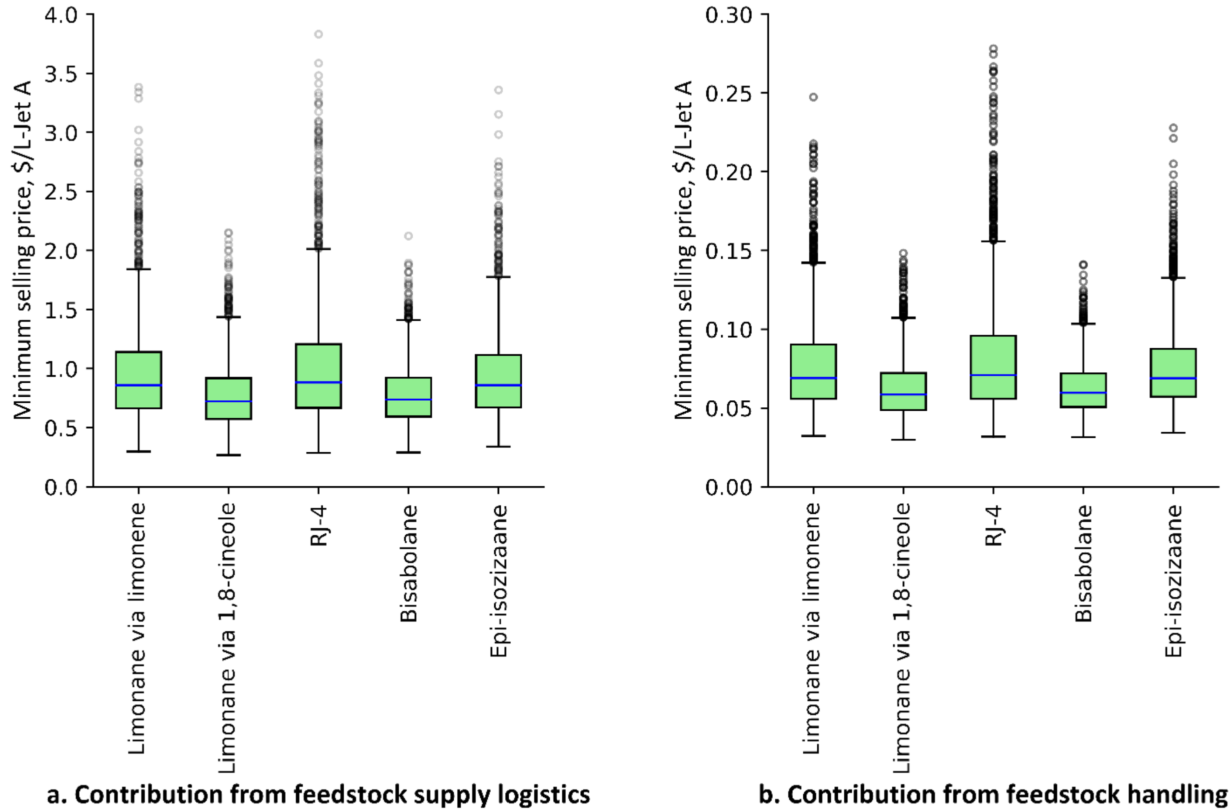
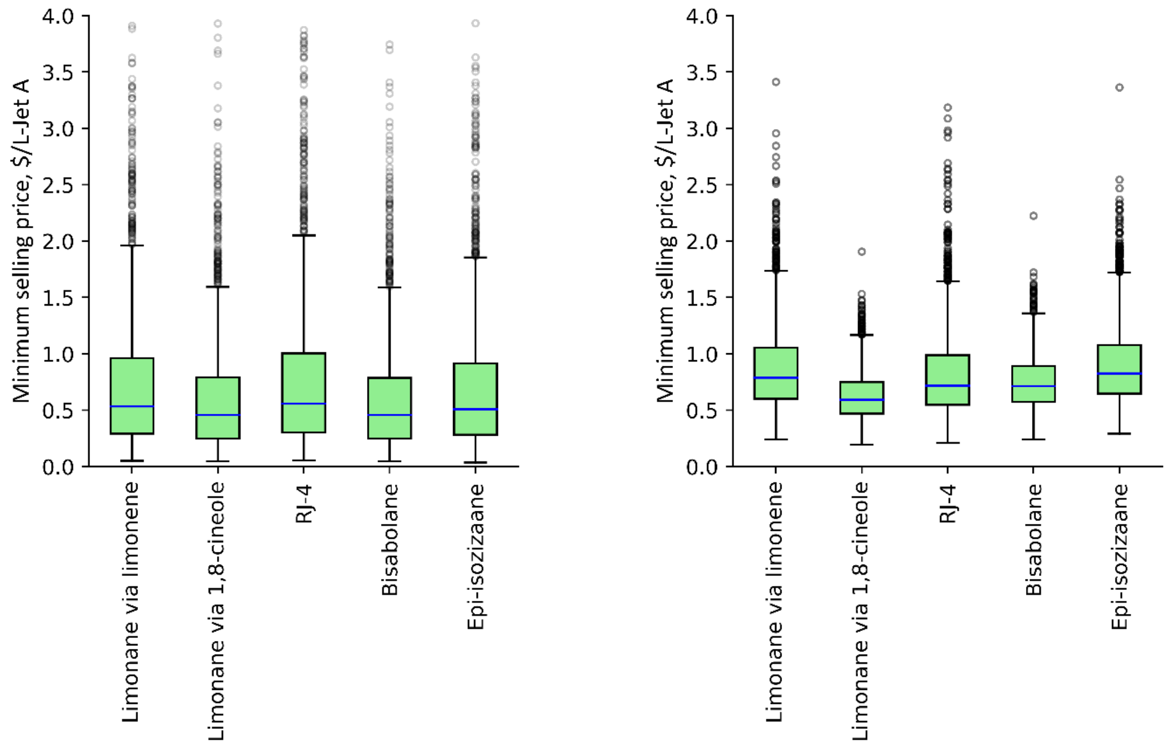


Figure S6. Uncertainty associated with feedstock supply (a) and handling (b) stages

S8.2 Pretreatment and Bioconversion



a. Contribution from biomass pretreatment **b. Contribution from hydrolysis and bioconversion**

Figure S7. Uncertainty associated with ionic liquid pretreatment (a), and aerobic bioconversion (b) stages

S8.3 Recovery and separation, and hydrogenation

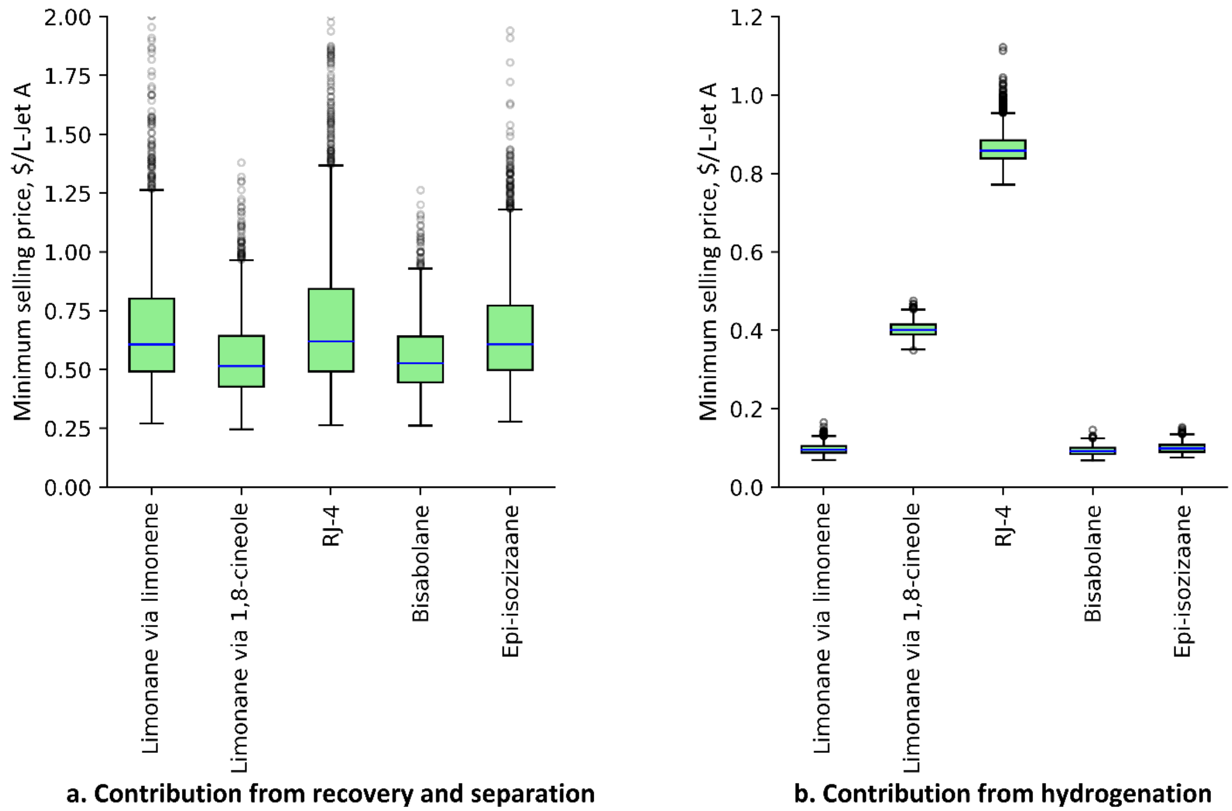


Figure S8. Uncertainty associated with recovery and separation (a) and hydrogenation (b) stages

S8.4 Wastewater treatment and onsite energy generation

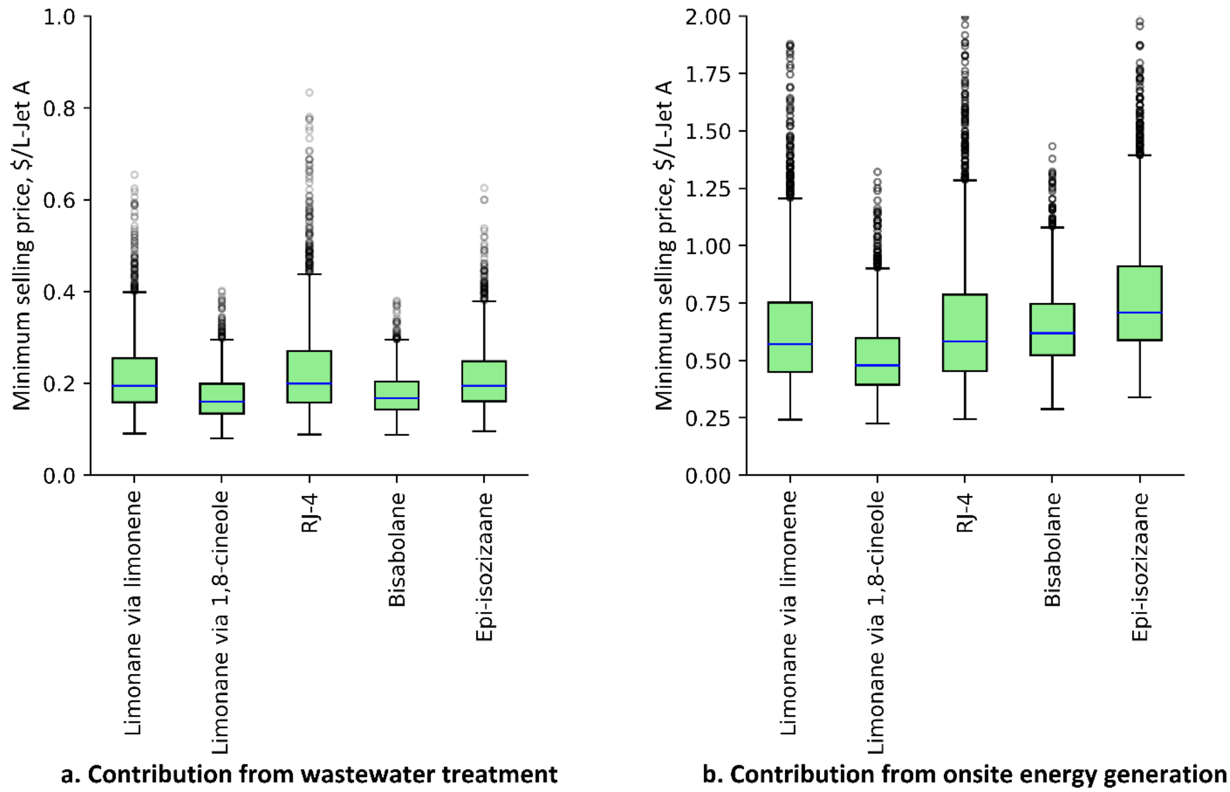


Figure S9. Uncertainty associated with wastewater treatment (a) and onsite energy generation (b) stages

S8.5 Minimum selling price of jet fuel

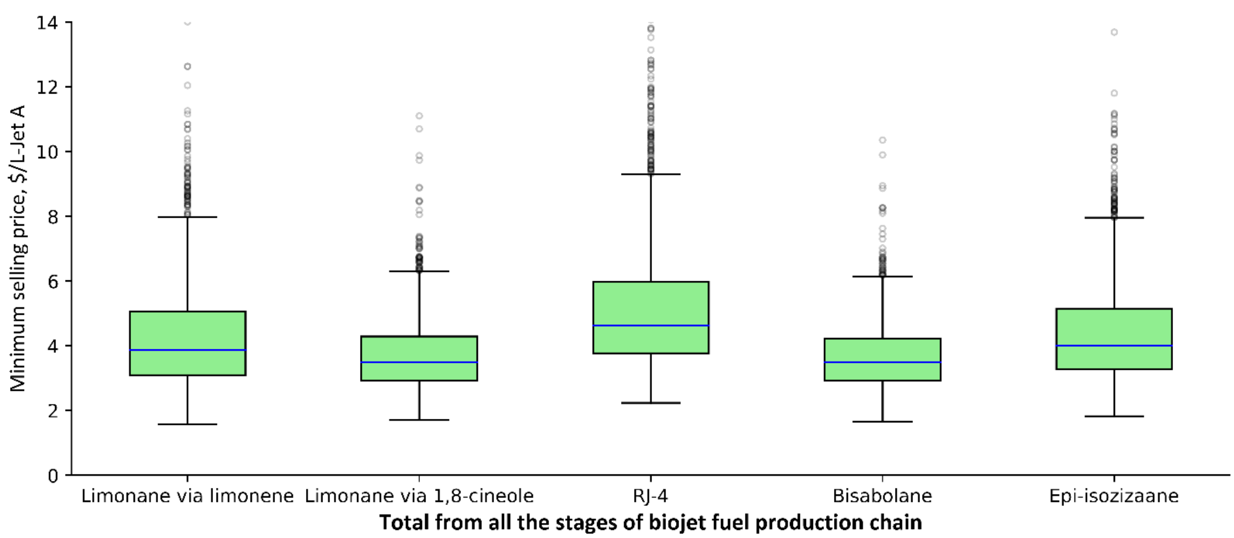
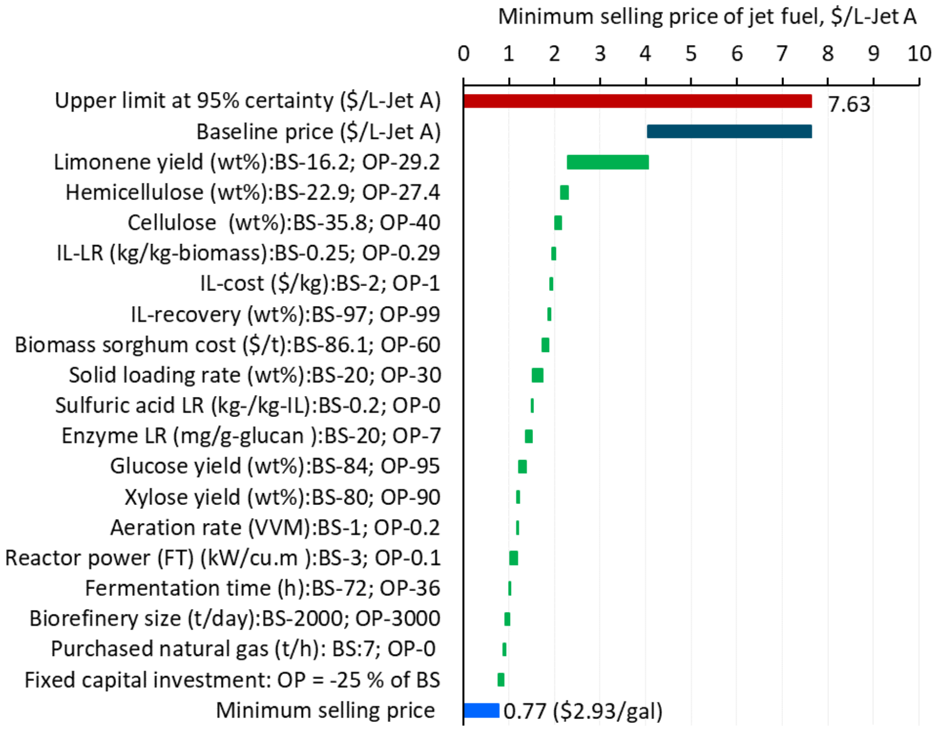


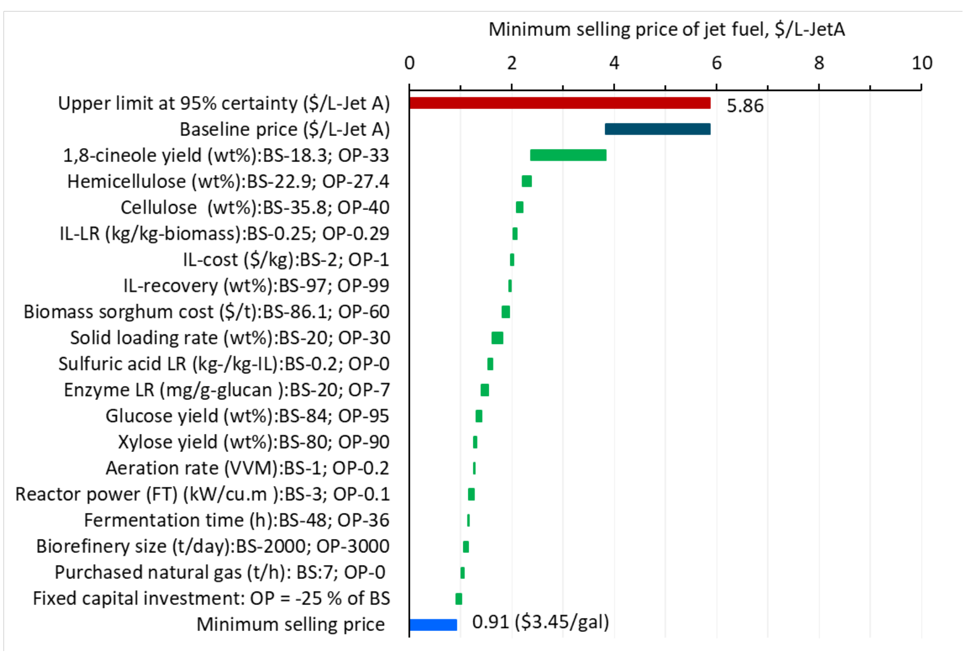
Figure S10. Uncertainty associated with the minimum selling price of different renewable jet fuel blendstocks

S9. Optimal minimum selling price of jet fuel

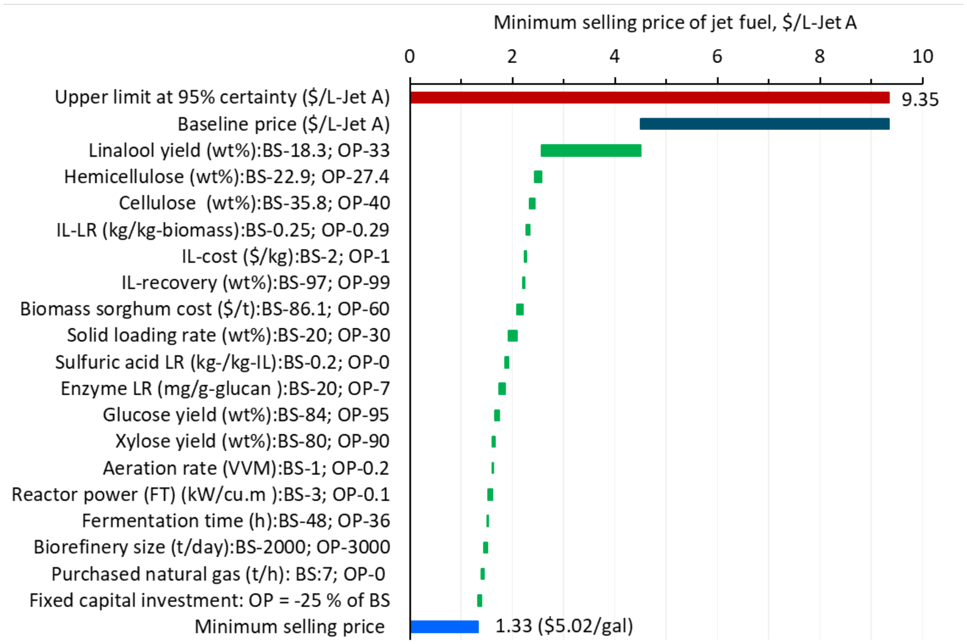
a. Limonane via limonene



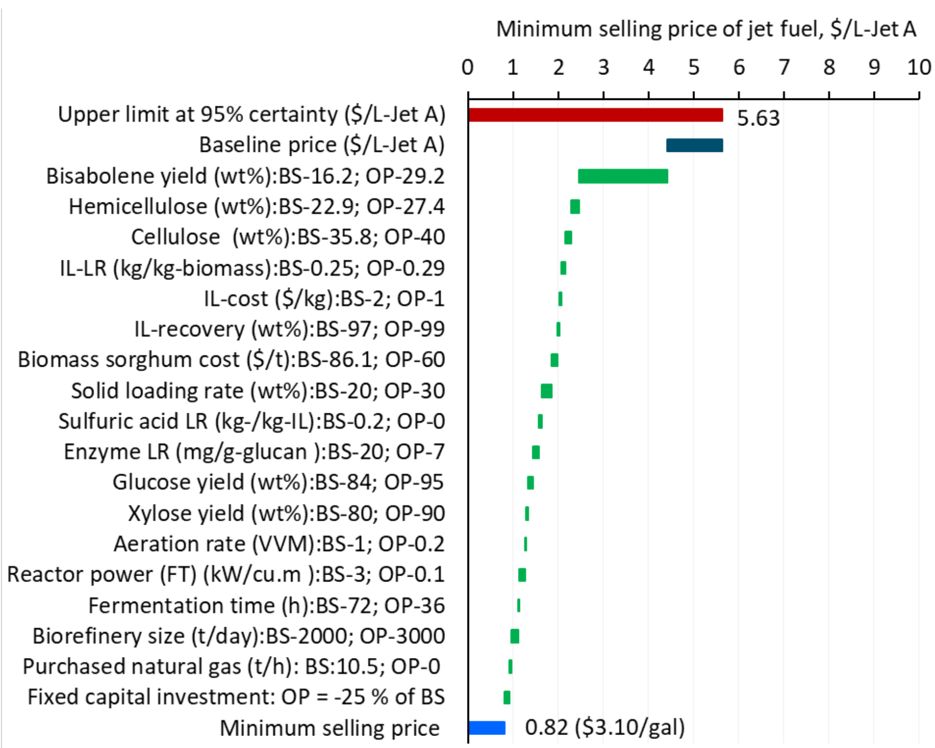
b. Limonane via 1,8-cineole



c. RJ-4



d. Bisabolane



e. Epi-isozizaane

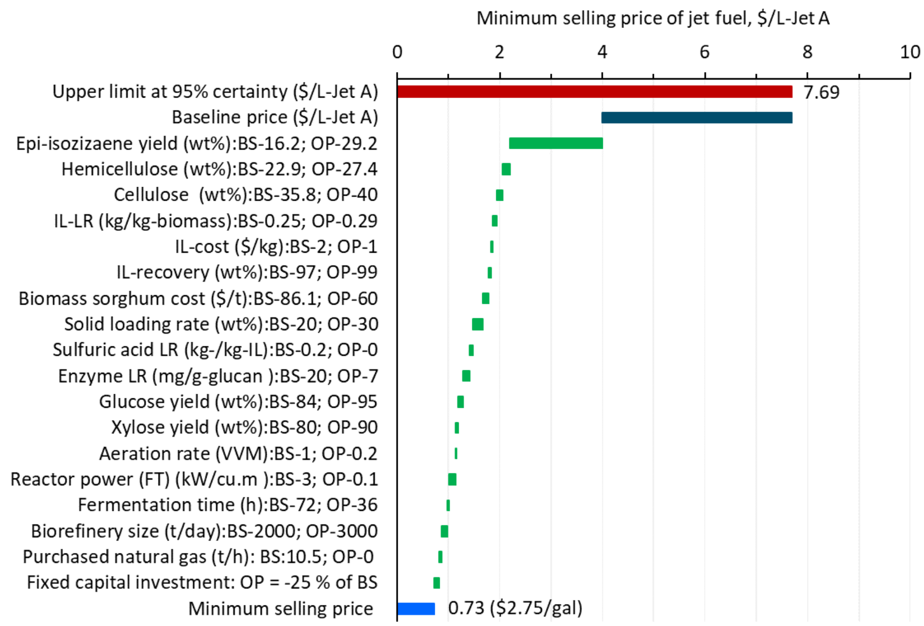


Figure S11. Step by step paths to reducing the minimum selling price of renewable jet fuel blendstocks. 'BC', 'LR' and 'IL' refer to bioconversion reactor, loading rate, and ionic liquid, respectively. 'BS' and 'OP' refer to baseline and optimal values, respectively.

S10. Future optimized selling price

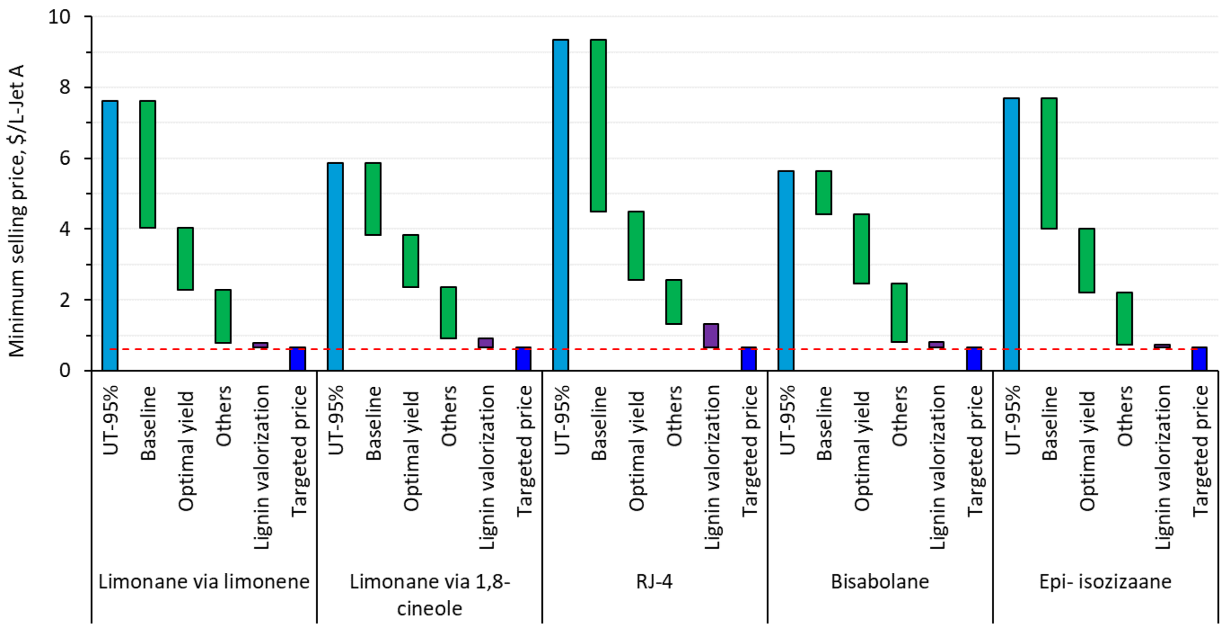


Figure S12. Paths to decreasing jet fuel selling prices. 'UL-95%' = upper limit of 95% confidence interval; 'Baseline' = Baseline Scenario (S2); 'Optimal yield' = 90% of the theoretical yield (S2); 'others' refer to the synergistic contribution of several input parameters, presented in (S8). Required lignin selling prices listed indicate The required selling prices of the hypothetical products to hit the targeted price of $0.66/L are $1.85, $2.1, $5.3, $1.9 and $1.9 per kg for limonane via limonene, limonane via 1,8-cineole, RJ-4, bisabolane, and epi-isozizaane, respectively. The horizontal dash line (- - - - - - -) refers to the last 10 years average Jet fuel selling price at refineries of 0.$61/L.[55]

S11. Comparison of greenhouse gas emissions from previous study

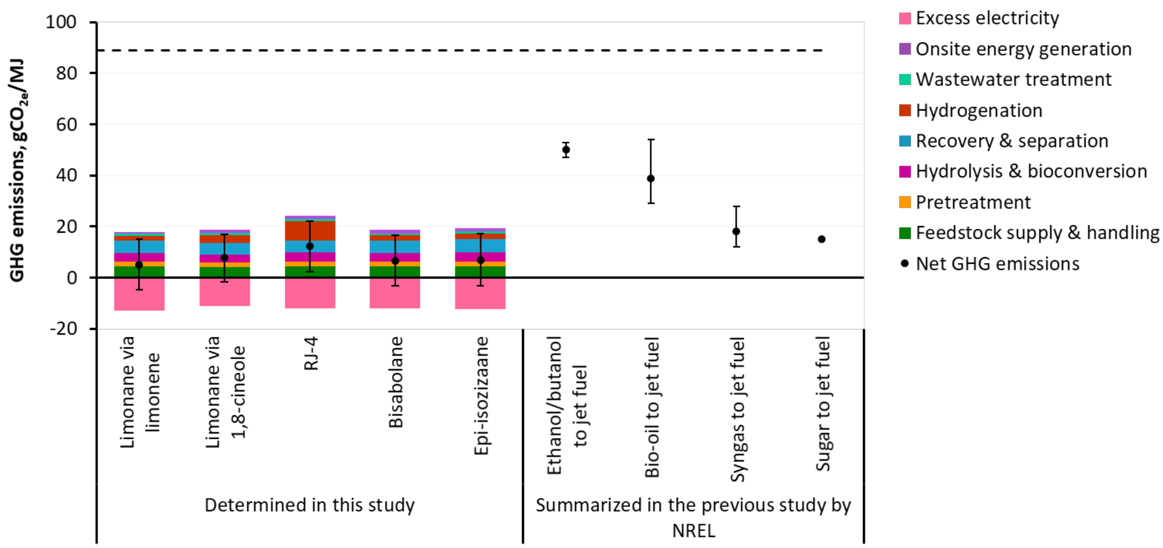


Figure S13. Greenhouse gas emissions associated with different renewable jet fuel molecules determined in this study for optimal future cases (S9). The horizontal dashed line (- - - - -) refers to the GHG emissions from conventional jet fuel of 89 gCO_{2e}/MJ. In this figure, the results from this study are compared with the results summarized in the previous review conducted by NREL. While the uncertainty bars in this study refers to the variation in the net GHG emissions due to the variability presents in the GHG emissions from land use changes, the higher- and lower-end uncertainties from the NREL study refers to the variability due to different feedstocks/conversion pathways. For the ethanol/butanol to jet fuel pathway, the higher- and lower-end uncertainties represent GHG emissions of n-butanol and ethanol, respectively. For the bio-oil to jet fuel pathway, represent GHG emissions of rapeseed and palm oils, respectively. Additionally, for the GHG emissions of bio-oil to jet fuel and syngas to jet fuel pathways, land use changes are not considered. Moreover, syngas to jet fuel pathways, switchgrass was selected as the feedstock; soil carbon sequestration was not considered. However, this study accounted for soil carbon sequestration of biomass sorghum feedstock and GHG emissions from land use changes.

S12. Uncertainty associated with net GHG emissions for the optimal future cases

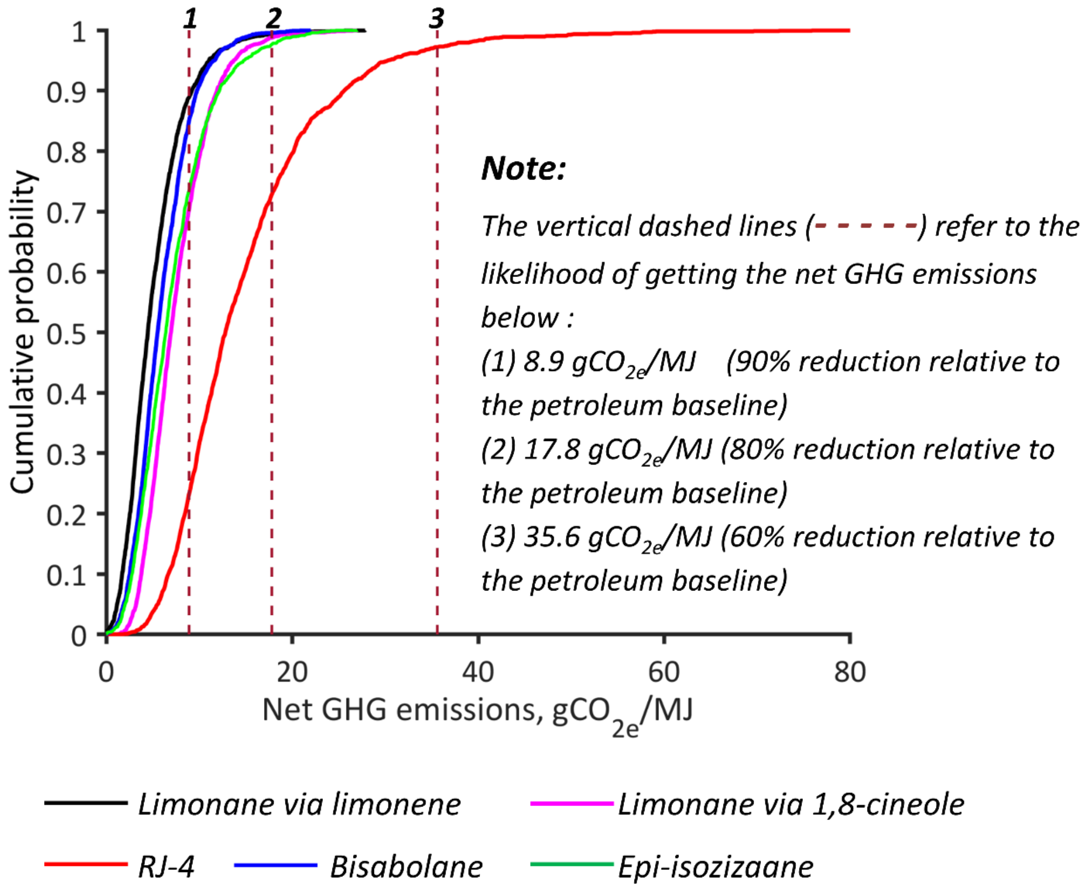


Figure S14. Likelihood of the net GHG emissions reduction below 60, 80, and 90% relative to the conventional jet fuel

S13. Major equipment cost per equipment type

Table S9. Major process equipment costs for limonane via limonene

Equipment Name	Equipment Sizing	Installation Factor	Unit Purchasing price (2018$)
Truck scale	Rated Throughput: 62998.96 kg/h	0.7	93,000
Truck dumper	Rated Throughput: 62998.96 kg/h	0.7	409,000
Truck dumper hopper	Rated Throughput: 62998.96 kg/h	0.7	424,000
Dust collection	Rated Throughput: 12599.79 kg/h	0.7	90,000
Belt Conveyor	Belt Length: 19.81 m	0.7	2,914,000
Silo/Bin	Vessel Volume: 27670.13 m^3	0.7	1,665,000
Belt Conveyor	Belt Length: 0.76 m	0.7	12,000
Belt Conveyor	Belt Length: 19.81 m	0.7	1,198,000
Shredder	Rated Throughput: 25199.58 kg/h	0.5	404,000
Flat Bottom Tank	Vessel Volume: 3.11 m^3	0.5	8,000
Centrifugal Pump	Power: 0.02 kW	2.1	8,000
Centrifugal Pump	Power: 5.45 kW	1.3	34,000
Centrifugal Pump	Power: 5.58 kW	1.3	34,000
Blending Tank	Vessel Volume: 0.89 m^3	1.5	6,500
Centrifugal Pump	Power: 0.07 kW	1.3	8,000
Stirred Reactor	Vessel Volume: 284.95 m^3	0.5	3,255,000
Receiver Tank	Vessel Volume: 207.02 m^3	1.6	91,000
Centrifugal Pump	Power: 0.01 kW	2.1	8,000
Centrifugal Pump	Power: 5.59 kW	1.3	35,000
Centrifugal Pump	Power: 7.9 kW	2.8	42,000
Centrifugal Pump	Power: 1.87 kW	1.3	22,000
Centrifugal Pump	Power: 7.47 kW	1.3	17,000
Flat Bottom Tank	Vessel Volume: 1517.81 m^3	0.7	446,000
Centrifugal Pump	Pump Power: 114.62 kW	1.3	122,000
Flat Bottom Tank	Vessel Volume: 2.65 m^3	0.7	13,000
Hopper	Vessel Volume: 23.62 m^3	1.6	76,000
Centrifugal Pump	Power: 0.02 kW	2.1	8,000
Centrifugal Pump	Power: 0 kW	1.3	8,000
Blending Tank	Vessel Volume: 23.62 m^3	1.5	82,000
Blending Tank	Vessel Volume: 1.8 m^3	1.5	7,000
Centrifugal Pump	Power: 1.01 kW	1.3	34,000
Centrifugal Pump	Power: 0.22 kW	2.8	17,000
Centrifugal Pump	Power: 0.32 kW	1.3	21,000
Heat Exchanger	Heat Exchange Area: 91.76 m^2	1.2	103,000
Component Splitter	Rated Throughput: 264600 kg/h	0.5	8,440,000
Pervaporation system	Rated Throughput: 179770.37 kg/h	0.5	56,034,000
Centrifugal Pump	Pump Power: 12.35 kW	1.3	50,000
Receiver Tank	Vessel Volume: 0.45 m^3	0.8	4,500
Centrifugal Pump	Power: 0.45 kW	1.3	12,000
Centrifugal Pump	Power: 1.03 kW	1.3	17,000
Clarifier	Surface Area: 224.82 m^2	0.5	3,570,000
Blending Tank	Vessel Volume: 0.06 m^3	1.5	5,500
Centrifugal Pump	Power: 1.64 kW	1.3	20,000
Flat Bottom Tank	Vessel Volume: 2803.43 m^3	0.51	282,000
Heat Exchanger	Heat Exchange Area: 99.06 m^2	1.2	108,000

Contd.

Table S9. Major process equipment cost (Contd.)

Equipment Name	Equipment Sizing	Installation Factor	Unit Purchasing price (2018$)
Centrifugal Fan	Rated Throughput: 183663 m^3/h	1	40,000
Centrifugal Pump	Pump Power: 3 kW	1.3	26,000
Component Splitter	Rated Throughput: 184.28 MT/h	0.61	1,563,000
Anaerobic digester	Rated Throughput: 225.84 MT/h	0.11	33,000,000
Aerobic bio-oxidation	Rated Throughput: 580.36 MT/h	1.07	1,727,000
Steam Generator	Throughput: 209.3 MT/h	0.8	26,547,000
Steam Turbine-Generator	Turbine Shaft Power: 77.04 MW	0.8	14,033,000
Centrifugal Pump	Pump Power: 25.17 kW	1.3	67,000
Heat Exchanger	Heat Exchange Area: 99.42 m^2	1.2	108,000
Centrifugal Compressor	Compressor Power: 889.1 kW	0.6	935,000
Blending Tank	Vessel Volume: 78.31 m^3	1.5	391,000
Centrifugal Pump	Power: 0.18 kW	1.3	17,000
Centrifugal Fan	Rated Throughput: 284078 m^3/h	1	56,000
Distillation Column	Column Volume: 4.13 m^3	1	102,000
Centrifugal Pump	Power: 3.88 kW	2.8	60,000
Heat Exchanger	Heat Exchange Area: 197.72 m^2	1.2	50,000
Centrifugal Fan	Rated Throughput: 569146.84 m^3/h	1	94,000
Component Splitter	Rated Throughput: 168.39 MT/h	0.5	8,440,000
Hydrotreating reactor	Vessel Volume: 33.33 m^3	0.5	3,808,000
Bioconversion reactor	Vessel Volume: 3485.21 m^3	0.5	2,181,000
Ultrafilter	Membrane Area: 77.21 m^2	0.5	119,000
Heat Exchanger	Heat Exchange Area: 196.67 m^2	1.2	50,000
Centrifugal Pump	Power: 1.9 kW	1.3	22,000
Decanter Centrifuge	Throughput: 342 m^3/h	0.5	233,000
Heat Exchanger	Heat Exchange Area: 184.41 m^2	1.2	48,000
Distillation Column	Column Volume: 12.9 m^3	0.5	127,000
Heat Exchanger	Heat Exchange Area: 94.62 m^2	0.5	105,000
Centrifugal Pump	Pump Power: 3.3 kW	1.3	28,000
Centrifugal Pump	Pump Power: 10.42 kW	1.3	47,000
Centrifugal Pump	Pump Power: 1.93 kW	1.3	22,000
Centrifugal Pump	Pump Power: 1.2 kW	1.3	18,000
Heat Exchanger	Heat Exchange Area: 35.73 m^2	1.2	59,000
Centrifugal Pump	Pump Power: 244.53 kW	0.5	165,000
Decanter Centrifuge	Throughput: 216.66 m^3/h	0.5	1,393,000

Note: Detailed specification of these process equipment are available in NREL's previous studies available at: https://www.nrel.gov/extranet/biorefinery/aspen-models/

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