Supporting Information: Catalytic Upgrading of Wet Waste-Derived Carboxylic Acids to Sustainable Aviation Fuel and Chemical Feedstocks

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Section S1. Interphase and Intraparticle Transport Limitations

Observed reaction rates were compared to maximum rates allowable by interphase and intraparticle mass and heat transport using the Mears[1] and Weisz-Prater[2] criteria. Mears' criterion for first-order reactions stipulates that an observed reaction rate is controlled by kinetics, not external mass or heat transport, if inequalities S1 and S2 are satisfied:

$$\frac{r''' r_p}{k_g C_{reactant}} < 0.15 \tag{S1}$$

$$\frac{|\Delta H| r''' r_p E_A}{h_t RT^2} < \frac{0.15RT}{E_A} \tag{S2}$$

In Inequalities S1-S2, r''' is the reaction rate per particle volume, r_p is the particle radius, k_g is the external mass transfer coefficient, $c_{reactant}$ is the bulk gas-phase concentration of reactant 4-heptanone, ΔH is the enthalpy of 4-heptanone at reaction conditions, E_A is the activation energy of 4-heptanone upgrading, h_t is the external heat transfer coefficient, R is the ideal gas constant (8.314 J mol^{-1} K^{-1}), and T is the absolute temperature of the reactor (623 K). We use a sample reaction of 4-heptanone upgrading to toluene and light alkanes to calculate enthalpy of reaction:

$$2\ C_7H_{14}O \rightarrow C_7H_8 + i\text{-}C_4H_8 + C_3H_6 + 2\ H_2O \tag{S3}$$

Values of all parameters are listed in Table S1. The external mass transfer coefficient is calculated according to the correlation developed by Wakao and Funazkri [3]:

$$k_g = \frac{D_{4-heptanone}}{D_{particle}}(2 + 1.1Re^{0.6}Sc^{0.33}) \tag{S4}$$

Values of all parameters are listed in Table S1. Here, $D_{4\text{-}heptanone}$ comes from the correlation developed by Fuller et al.[4]

$$D_{4-heptanone,He} = \frac{10^{-7}T^{1.75}\left(\dfrac{1}{MW_{4-heptanone}} + \dfrac{1}{MW_{He}}\right)^{0.5}}{P\left(v_{4-heptanone}^{\frac{1}{3}} + v_{He}^{\frac{1}{3}}\right)^2}$$

Here, T is absolute reaction temperature (623 K), $MW_{4\text{-}heptanone}$ and MW_{He} are the molecular weights of both species, P is the pressure in atmospheres (1.6), and $v_{4\text{-}heptanone}$ and v_{He} are the diffusion volumes of both species, 230.54 and 2.88 respectively. Re, the particle Reynolds number, is calculated according to the formula:

$$Re = \frac{D_{particle}\dot{m}}{\mu A \nu_{reactor}}$$
(S5)

Reynolds numbers are calculated for both liquid and gas films. The total mass flow through the reactor ($\dot{m}$) is computed according to the mixture properties detailed in the experimental section (total 4-heptanone and helium influent), mixture viscosity (μ) is calculated using the Wilke gas mixture visocosity formula for the gas phase[5], with individual component viscosities at reaction conditions tabulated in the NIST/TRC Web Thermo Tables[6], and reactor cross-sectional area ($A_{reactor}$) for the 0.0047 m inner diameter tube described in the experimental section is used. The formula for Sc, the Schmidt number, is:

$$Sc = \frac{\mu}{\rho D_{particle}}$$
(S6)

All parameter values are listed in Table S1. The mass density of the reaction mixture (ρ) calculated using the ideal gas law. The external heat transfer coefficient, h_t, is computed using the correlation developed by De Acetis and Thodos:[7]

$$h_t = \frac{\lambda}{D_{particle}} * 0.023 Re^{0.8} Pr^{0.8}$$
(S7)

The thermal conductivity of the reaction mixture, λ, is calculated using the Wilke gas mixture thermal conductivity formula[5], with individual component viscosities at reaction conditions tabulated in the NIST/TRC Web Thermo Tables.[6] Pr, the Prandtl number, is calculated from:

$$Pr = \frac{\mu C_p}{\lambda}$$
(S8)

The mixture heat capacity (C_p) is a mass-weighted average of all individual component heat capacities at reaction conditions tabulated in the NIST/TRC Web Thermo Tables.[6] The left side of Inequality S1 in the liquid film case is $9.6*10^{-2}$, meaning mass transfer is not limited in film of gas around the particle. The left side of Inequality S2 is $1.5*10^{-3}$ and the right side is $3.9*10^{-3}$, so we conclude that no significant temperature gradient exists between the bulk fluid of the reactor and the catalyst surface.

If the Weisz-Prater criteria (Inequalities S9-S10) are satisfied, reaction rates are not limited by internal heat or mass transport:

$$\frac{r''' r_{particle}^2}{D_{pore} c_{reactant}} < 1$$
(S9)

$$\frac{\Delta H r''' r_p^2}{\lambda_{particle} T} < \frac{0.75 RT}{E_A}$$
(S10)

D_{pore}, the pore diffusion coefficient, is a combination of free ($D_{4\text{-}heptanone}$) and Knudsen ($D_{Knudsen}$) diffusion resistances for hexadecane, corrected for particle tortuosity (τ) and porosity (ε):

$$D_{pore} = \frac{\epsilon}{\tau}\left(\frac{1}{\frac{1}{D_{4-heptane}} + \frac{1}{D_{Knudsen}}}\right)$$
(S11)

Table S1 lists typical ε and τ values for a typical highly tortuous zeolite, as well as the Knudsen diffusion, calculated according to the formula listed in Davis and Davis:[8]

$$D_{Knudsen} = 0.97 * \frac{r_{pore}}{10^8} \sqrt{\frac{T}{MW_{4-heptane}}}$$

(S12)

Equation S12 utilizes the pore radius of H/ZSM-5 (r_{pore}) and the molecular weight of hexadecane ($MW_{4-heptanone}$). These values, along with the thermal conductivity of a typical zeolite ($\lambda_{particle}$) from Schnell and Vlugt [9] are listed in Table S1. Since the value of the left side of Inequality S9 is 9.8, the reaction is limited by internal molecular diffusion limitations, as expected. However, the value of the right side of Inequality S10 is $8.4*10^{-6}$ while the value of the left side is $1.9*10^{-2}$, so no significant thermal gradients exist within zeolite particles.

Table S1. Parameters used in Mears and Weisz-Prater criterion calculations.

Parameter	Value	Source
r'''	3.5 mol m^{-3} s^{-1}	Maximum site-time yield for 4-heptanone upgrading observed at partial conversion; $\rho_{particle}$=0.4 g cm^{-3}
r_p	400 μm	40 mesh particle
k_g	$4.9*10^{-3}$ m s^{-1}	Wakao and Funazkri [3]
$c_{reactant}$	2.97 mol m^{-3}	Ideal gas law
ΔH	+22.5 kJ mol^{-1}	NIST/TRC Web Thermo Tables [6]
E_A	200 kJ mol^{-1}	Reasonable upper limit; lower values of E_A only make both Mears and Wesiz-Prater heat transfer criteria more flexible
h_t	2.77 W m^{-2} K^{-1}	De Acetis and Thodos [7]
$D_{4-Heptanone}$	$4.2*10^7$ m^2 s^{-1}	Fuller et al.[4]
Re	0.26	
Sc	170	
$\dot{m}$	$3.6*10^{-7}$ kg s^{-1}	Experimental section
μ	$3.2*10^{-5}$ kg m^{-1} s^{-1} (gas)	NIST/TRC Web Thermo Tables;[6] Wilke[5]
$A_{reactor}$	$1.7*10^{-5}$ m^2	Experimental section
ρ	0.45 kg m^{-3} (gas)	Experimental section
λ	$1.9*10^{-3}$ W m^{-1} K^{-1}	NIST/TRC Web Thermo Tables;[6] Wilke [5]
Pr	0.27	
C_p	2.0 kJ kg^{-1} K^{-1}	NIST/TRC Web Thermo Tables;[6] Experimental section
D_{pore}	$4.8*10^{-9}$ m^2 s^{-1}	

$D_{Knudsen}$	$1.2*10^{-7}$ m^2 s^{-1}	
ε	0.5	
τ	10	
$\lambda_{particle}$	0.6	Schnell and Vlugt [9]
r_{pore}	5.5 Å	
$MW_{4\text{-}Heptanone}$	114.19 g mol^{-1}	

Section S2. Supplementary Experimental Methods

Figure S1 shows the X-ray diffractogram of the H/ZSM-5 sample used for ketone cyclization in this work. Specific surface areas of all catalysts tested for 4-heptanone conversion are shown in Table S2.
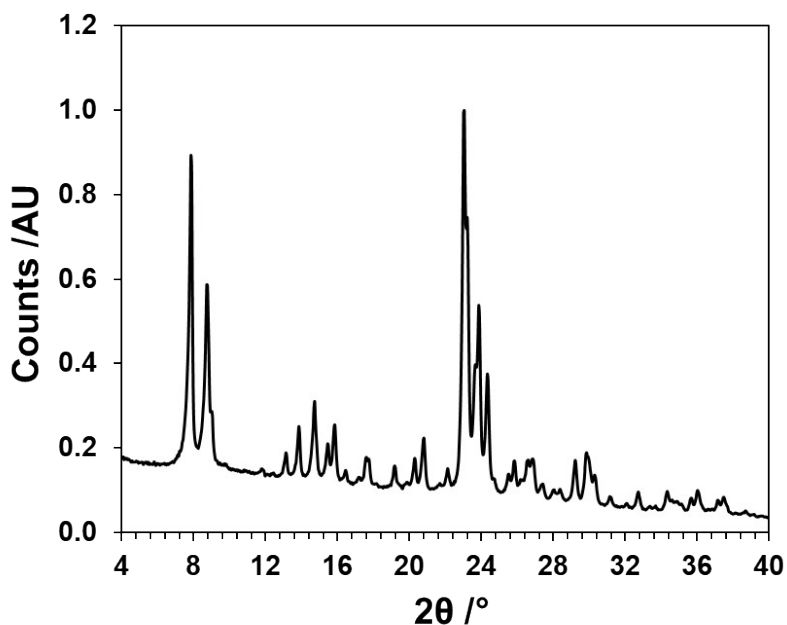

Figure S1. X-ray diffractogram of Zeolyst CBV8014 ZSM-5 (Si:Al=40) used in this work.

Table S2. Specific surface areas of all catalysts tested for 4-heptanone conversion using calculated using BET analysis of N$_2$ physisorption isotherms.

Sample	Surface area /(m^2/g)
ZrO$_2$	52
TiO$_2$	60
Niobic acid	74
Mg$_6$Al$_2$O$_8$	135
H/ZSM-5	403
H/BEA	1103
H/FAU	1352
H/MOR	561

Coke deposition on H-ZSM/5 for catalyst oxidative regeneration procedure development was analyzed using a Setaram Setsys Evolution TGA instrument. A gas flow of 50 sccm zero air was fed continuously through the TGA chamber. The system was held at 20°C for 10 min after loading as a stabilization step followed by a temperature ramp of 10°C min^{-1} to 120°C, where it was held for 30 min to remove moisture. Then the temperature was ramped at 20°C min^{-1} to 550°C, where it was held for 4h. A final temperature ramp was conducted at 20°C min^{-1} to reach 800°C, where the temperature program ended, and the sample promptly started cooling to 20°C. In a second experiment, after the drying step, the temperature was ramped directly to 800°C at 20°C min^{-1}, where the temperature program ended, and the sample promptly started cooling to 20°C.

Heteroatom impurity content of aqueous and solid samples was determined by first mineralizing 250 mg in a quartz tube with 4 mL of concentrated nitric acid using a microwave digestion system (UltraWAVE 2, Milestone) at 1500 W following the UW-GE-4 method provided by Milestone. These samples were then diluted to 50 mL distilled water with 0.25 mL of 1000ppm yttrium in 2% nitric acid (Accustandard; New Haven, CT) added to serve as an internal standard.

These diluted samples were than analyzed via inductively coupled plasma optical emission spectrometer (ICP-OES 5100; Agilent Technologies Inc.). The method conditions and element wavelengths are listed in Table S3 below.

Table S3. ICP-OES parameters for aqueous and solid samples.

ICP-OES Parameter	Setting
Read time	20
RF Power (kw)	1.40
Stabilization time (s)	15
Viewing Mode	Axial
Viewing height (mm)	8
Nebulizer flow (L/min)	0.60
Plasma flow (L/min)	13.0
Aux flow (L/min)	1.00
Make-up flow (L/min)	0.00
Elements	Al (396.152 nm); Ca (315.887 nm); Fe (238.204); K (766.491 nm); Mg (285.213 nm); Mn (257.610 nm); Na (589.592 nm); P (213.618 nm); S (181.972 nm); Zn (206.200 nm)

Similarly, heteroatom impurity content of organic samples was determined by first mixing 500 mg of sample into a 50 mL centrifuge tube and diluted to 25 mL with diglyme (Sigma Aldrich; St. Louis, MO) and 0.5 mL of 40ppm yttrium in 2% nitric acid. These samples were then vortexed to assure complete homogeneity.

These diluted samples were than analyzed via inductively coupled plasma optical emission spectrometer (ICP-OES 5100; Agilent Technologies Inc.). The method conditions and element wavelengths are listed in Table S4 below.

Table S4. ICP-OES parameters for organic samples.

ICP-OES Parameter	Setting
Read time	40
RF Power (kw)	1.40
Stabilization Time (s)	25

Viewing Mode	Axial, Radial (-R)
Viewing height (mm)	8
Nebulizer flow (L/min)	0.50
Plasma flow (L/min)	16
Aux flow (L/min)	1.00
Make-up flow (L/min)	0.00
Oxygen (%)	25
Elements	Al (396.152 nm); B (208.956 nm); Ca (393.366 nm); Fe (238.204 nm); K-R (766.491 nm); Mg-R (279.553 nm); Mn (293.305 nm); Na (588.995 nm); P (213.618 nm); S (180.669 nm); Si (288.158 nm); Zn (206.200 nm)

Properties of the Jet A sample used for blending with the bioblendstock and ASTM test methods used in measuring these properties are listed in Table S5.

Table S5. Properties of the Jet A sample used for blending with bioblendstock and ASTM test methods used to measure these properties. Surface tension (not shown here) was measured using ASTM D1331.

Property	Test Method	Value
Distillation	D2887 (D86 correlation)	
T10, °C		183
T50, °C		215
T90, °C		262
Final boiling point, °C		291
Flash point, °C		48.6
Density at 15°C, kg/m^3	D7042	802.0
Freezing point, °C	D5972	-45.9
Cetane Number (as ICN)*		48.8
Viscosity at -20°C, mm^2/s	D7042	4.745
Viscosity at -40°C, mm^2/s	D7042	9.789
Surface tension at 20°C, mN/m	D1331	25.77
Net heat of combustion (higher heating value), MJ/kg	D240	43.14
Carbon, wt%	D5291	86.608
Hydrogen, wt%	D5291	13.814
Nitrogen, wt%	D5291	0.0153

* Indicated cetane number (ICN) has been shown to be equivalent to derived cetane number (DCN), which is currently the method required in D4054.[10]

Section S3. Supplementary Experimental Tables and Figures

Figures S2-6 show reaction, themogravimetric analysis, and impurity analysis data for various VFA and ketone upgrading steps. Table S6 shows impurity analysis of all stages of food waste-derived acids upgrading to SAF and chemical precursors. Figure S7 shows mass tracking in upgrading of food waste-derived salts.
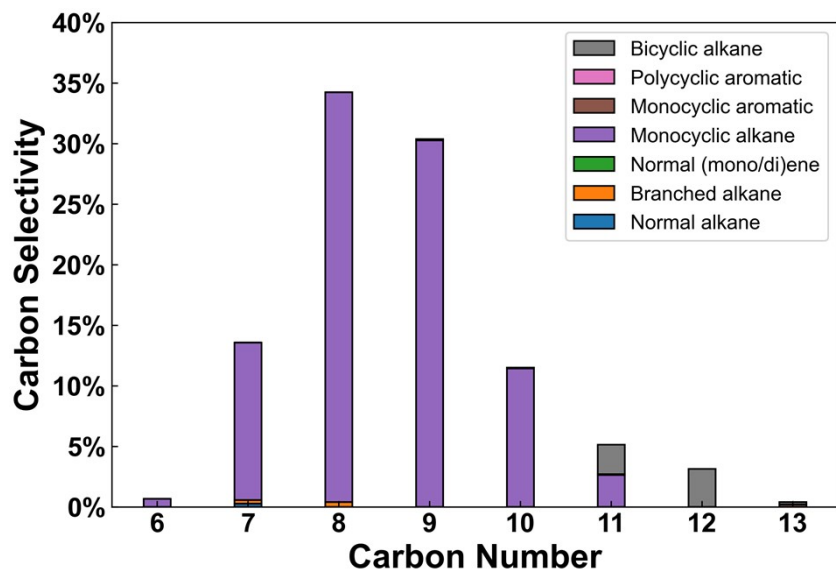
Figure S2. Saturation over Pd/Al$_2$O$_3$ of aromatic-heavy mixture from 4-heptanone upgrading. Reaction conditions: T: 200°C, P$_{H2}$=3500 kPa, WHSV=0.24 hr^{-1}, m$_{Catalyst}$=4 g.
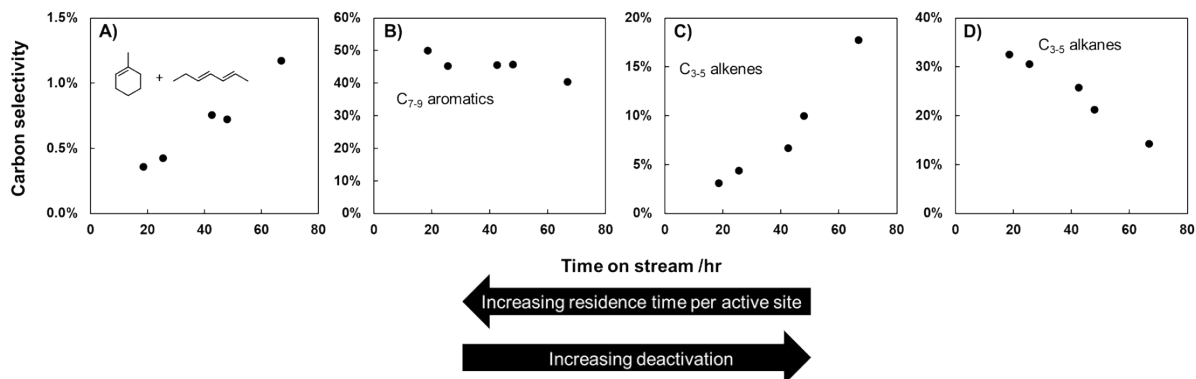

Figure S3. Product selectivities plotted as a function of time on stream in 4-heptanone upgrading over H/ZSM-5 (Si/Al=40) at over 100% 4-heptanone conversion. Reaction conditions: T: 350°C, P$_{Total}$=130-170 kPa, P$_{4-Heptanone}$=13-17 kPa, balance He (30 sccm), WHSV=0.95 hr^{-1}, m$_{H/ZSM-5}$=1 g.
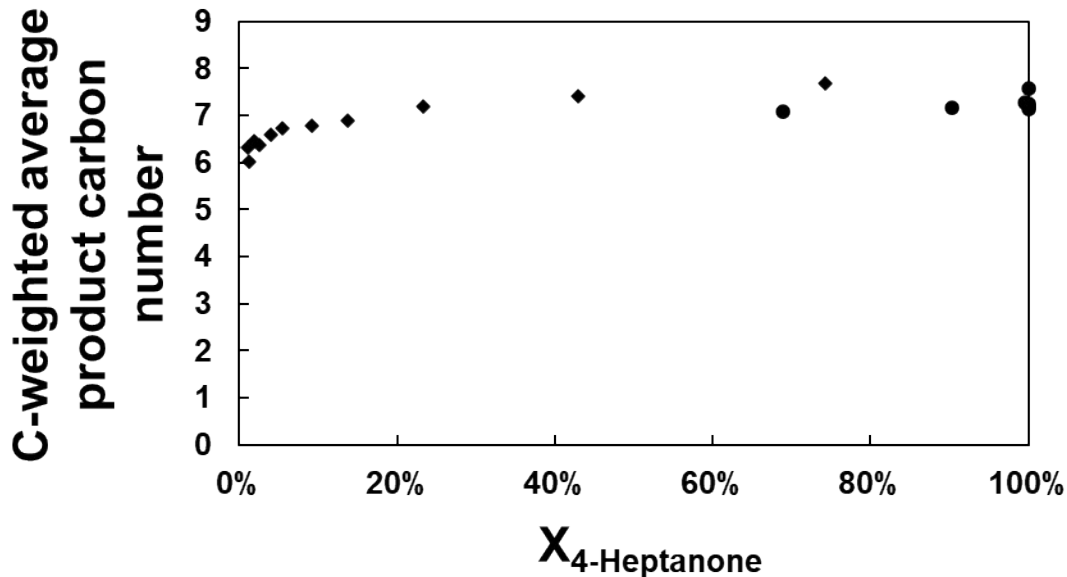
Figure S4. Carbon-weighted average carbon number (dot product of vectors of product carbon selectivities and carbon numbers) of 4-heptanone upgrading products at varied 4-heptanone conversion. Conversion was modulated via catalyst deactivation with time on stream. Different symbols correspond to different experiments. Reaction conditions: T: 350°C, PTotal=130-170 kPa, P4-Heptanone=13-17 kPa, balance He (30 sccm), WHSV=1-2 hr-1, mH/ZSM-5=0.5-1 g, selectivities measured between 20-165 hours on stream.
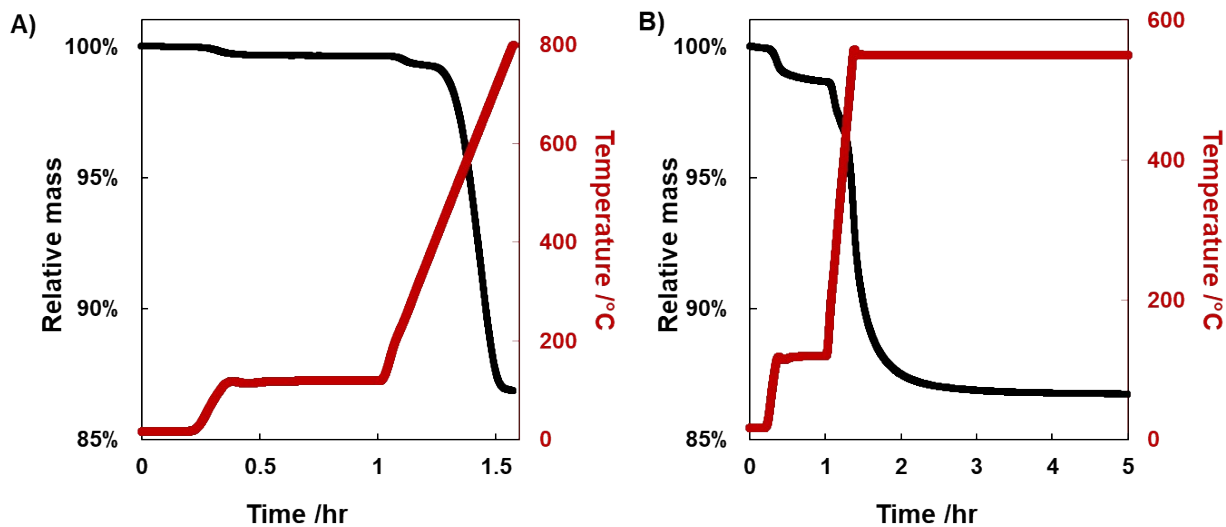

Figure S5. Thermogravimetric analysis (TGA) of catalysts used for 4-heptanone upgrading at 350°C for 165 (A) or 48 (B) hours on stream. Conditions: 50 sccm air flow.
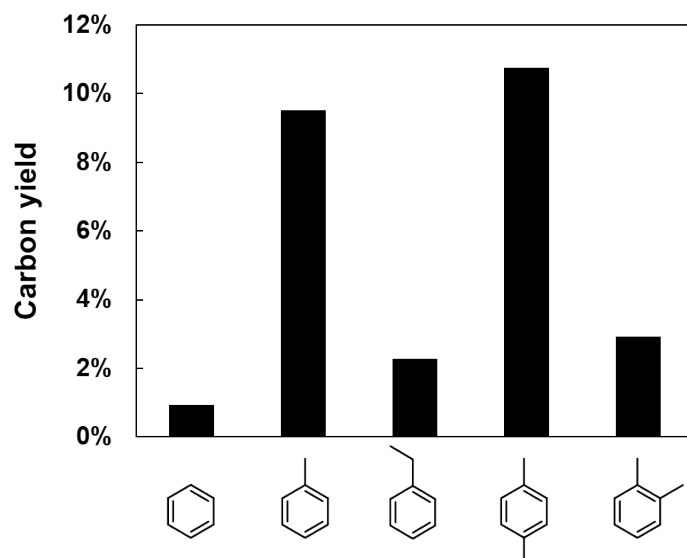
Figure S6. Yields of individual BTEX compounds (in order of appearance: benzene, toluene, ethyl benzene, p-xylene, and o-xylene) during upgrading of food waste-derived light ketones over H-ZSM/5. Reaction conditions: T=350°C, P_{total}=180 kPa, He flow=30 sccm, WHSV=0.86 hr^{-1}, $m_{H/ZSM-5}$=4.0 g.
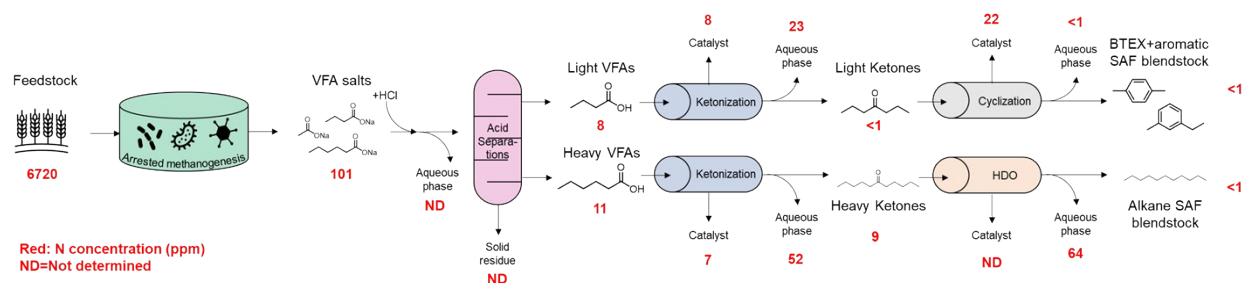
Figure S7. Nitrogen content of reactants, intermediates, products, and catalysts associated with every step of food waste upgrading to SAF, BTX, and other hydrocarbons.

Table S6. Metal, halogen, N, P, B, and S concentrations in VFA salt feed, final products, intermediates, aqueous byproducts, and catalysts used in food-waste derived VFA upgrading to SAF, BTEX, and light hydrocarbons. ND=not detected.

|	N	Total Halogens	Al	B	Ca	Co	Cr	Fe	K	Li	Mg	Mn	Na	Ni	P	S	Sr	Zn
ChainCraft Salts	101	1050	86.16	ND	731.33	<10	<10	27	1836	10	413	<10	159051	<10	152	403	<10	<10
Separated VFAs																		
Light VFAs	8	<10	<3	6.03	11.02	ND	ND	<10	2274.25	<10	268.06	ND	1971.33	ND	37.88	ND	22.93	<2
Heavy VFAs	11	<10	4.06	<2	<2	ND	ND	<10	<2	<10	<2	ND	16.1	ND	<2	ND	<2	5.12
Ketonization																		
Light Ketones	<1	<10	4.65	4.5	<2	ND	ND	<10	<2	ND	<2	ND	<2	ND	<2	ND	<2	3.05
Light Ketones-Aqueous	23	<10	39.87	ND	175.83	<10	<10	<10	37.17	<10	16.54	ND	381.27	ND	11.37	ND	<10	<10
Light Ketones-ZrO$_2$	8	100	377.73	ND	345.13	<10	66.73	5667.09	26897.57	<10	2831.42	208.54	20780.44	96.34	<10	<10	237.13	<10
Heavy Ketones	9	<10	4.02	4.66	<2			<10	<2	<10	<2		4.79		<2		<2	3
Heavy Ketones-Aqueous	52	<10	38.54	ND	161.81	<10	<10	<10	35.05	<10	14.07	<10	387.59	<10	10.88	<10	<10	<10
Heavy Ketones-ZrO$_2$	7	480	101.92	ND	234.7	18.56	2963.1	5667.09	26897.57	<10	2831.42	337.49	2578.39	62.61	<10	<10	<10	<10
Hydrocarbon formation																		
Aromatics	<1	<10	<3	<2	<2	ND	ND	<10	<2	<10	<2	ND	<2	ND	<2	ND	<2	<2
Aromatics-Aqueous	<1	<10	36.83	ND	142.39	<10	<10	<10	37.26	<10	12.69	<10	418.08	<10	<10	<10	<10	<10
Aromatics-H/ZSM-5	22	<10	1306.83	ND	197.43	<10	<10	212.17	36.57	11.2	58.67	<10	383.88	10.39	13.61	<10	<10	<10
Alkanes	<1	<10	<3	<2	<2	<2	<2	<2	<2	<2	<2	<2	3	<2	<2	<2	<2	<2
Alkanes-Aqueous	64	<10	37.74	ND	173.08	<10	<10	<10	37.95	ND	10.25	<10	413.12	<10	10.49	<10	<10	<10
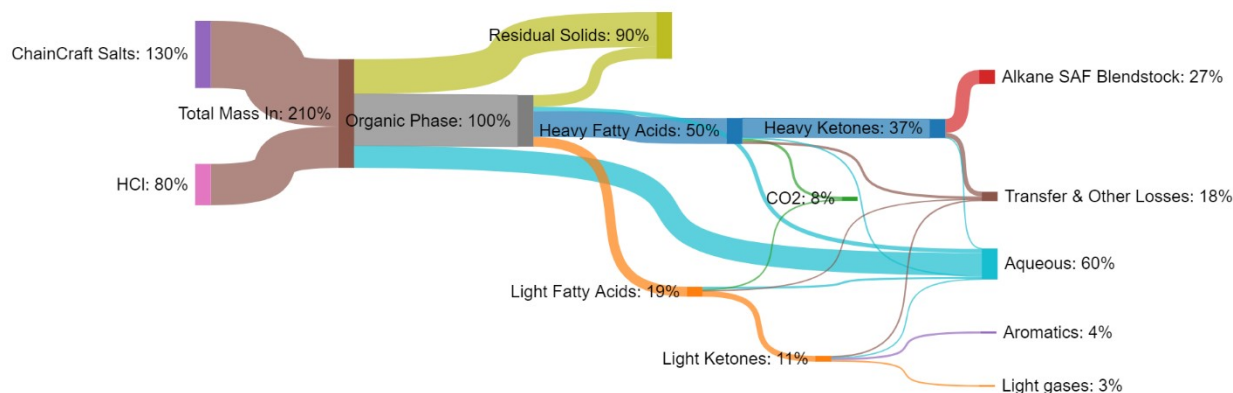
Figure S8. Mass flows to SAF precursors and other side products during upgrading of ChainCraft acid salts to SAF blendstock and chemical precursors. Mass losses from a spill which occurred while preparing for ketone hydrotreating are not included.

Section S3. Techno-economic analysis and life-cycle assessment information

The process design for the TEA and LCA model, shown in Scheme 1, is similar to designs in our previous work. The utilities and front-end VFA production operations (arrested anaerobic digestion and in situ product recovery) are consistent with those modeled in Wiatrowski et al.[11] and most upgrading operations (VFA distillation, ketonization, and hydrotreating) are consistent with the model described in Miller et al.[12] The exception is the cyclization reaction and separation approach, which has not been included in our previous work and will be described here in more detail.

Ketones are fed to a moving bed reactor over a H/ZSM-5 catalyst (weight hourly space velocity [WHSV] of 1 hr^{-1}, 350°C, in 90 mol% N_2). Catalyst is continuously removed from the bottom of the reactor and regenerated with 1% O_2 in a design resembling the continuous catalyst regeneration (CCR) process by Honeywell UOP.[13] Following reaction, the mixture hydrocarbons is separated into products (BTEX, SAF, naphtha) and light gases (combusted for energy recovery). The modeling and costing details for the separations portion of cyclization were adapted from Yadav et al.[14] The gaseous mixture is first fed to the bottom of an extractive distillation column utilizing a sulfalone solvent, with light alkanes removed in the distillate. The bottoms stream of the first column is then fed to a solvent recovery column, and the resulting bottoms stream (consisting of sulfolane and some heavier aromatics) is recycled to the top of the extractive distillation column (a 1% purge is removed to prevent buildup of heavier aromatics). The distillate from the solvent recovery column is decanted to remove water before being fed to a final distillation column to separate out the BTEX (to the distillate) and remaining SAF-range components (to the bottoms).
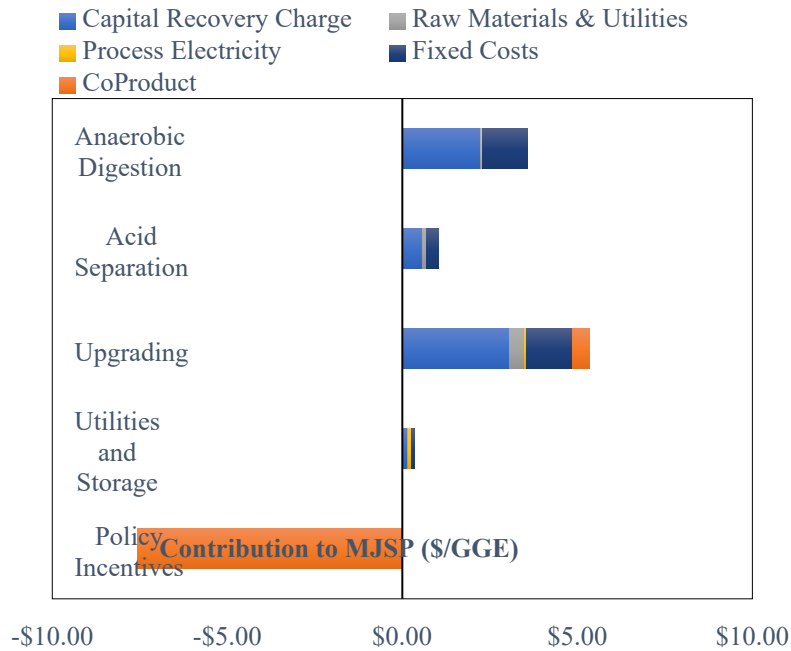
Figure S9. Cost breakdown of the MJSP from the TEA model.

Table S7. Summary of capital expenditures in the TEA model.

Total Direct Costs (TDC)	$15,914,000
Total Installed Cost	$15,246,000
Inside Battery Limits (ISBL)	$14,837,000
Outside Battery Limits (OSBL)	$409,000
Additional Piping (4.5% of ISBL)	$668,000
Total Indirect costs	$3,183,000
Project Contingency (10% of TDC)	$1,591,000
Other Costs (Start-Up, Permits, etc.) (10% of TDC)	$1,591,000
Fixed Capital Investment	$19,096,000
Land	$700,000
Working Capital (5% of FCI)	$955,000
Total Capital Investment	$20,751,000

Table S8. Summary of fixed costs for the TEA model.

Labor and Supervision	
Operations Salaries	$505,670
Maintenance Salaries	$195,539
Total Salaries	$701,208
Labor Burden (90%)	$631,088
Other Overhead	
Maintenance	$445,106
Property Insurance and Taxes	$133,675
Total Fixed Costs	**$1,911,077**

Table S9. Financial assumptions and design basis used for the TEA model.

Financial Assumptions	
Plant life	30 years
Plant throughput	250 wet tons per day (food waste)
Cost year dollar	2020
Capacity Factor	90%
Discount rate	10%
General plant depreciation	MACR
General plant recovery period	7 years
Steam plant depreciation	MACR
Steam plant recovery period	20 years
Federal tax rate	21%
Financing	40% equity
Loan terms	10-year loan at 8% APR
Construction period	3 years
First 12 months' expenditures	8%
Next 12 months' expenditures	60%
Last 12 months' expenditures	32%
Working capital	5% of fixed capital investment
Start-up time	6 months
Revenues during start-up	50%
Variable costs during start-up	75%

Table S10. Modeled Policy Incentive Values, Length of Duration, and Minimum GHG Reduction.

Policy Incentive	Base Value	Duration (years)	Minimum GHG Reduction	Reference
LCFS Credits	$133/tonne CO_2 reduction	Life of plant	50%	California LCFS; 6-year average (2014-2019).
D5 RIN credits	$0.81/gal ethanol equivalent	Life of plant	50%	Renewable Fuel Standard; 6-year average (2016-2021)

	(applies to all liquid fuels)			
SAF blender's tax credit	$1.25-$1.75/gal SAF [a]	4	50-100%	26 U.S. Code § 6426 & 40B
Alternative fuel mixture credit	$0.50/gal naphtha	4	50%	26 U.S. Code § 6426 & 40

[a] SAF blender's tax credit varies linearly based on GHG reduction; $1.25/gal is applied at a 50% GHG reduction, with an additional $0.01/gal credit applied for each percentage point reduction up to a maximum of $1.75/gal at 100% GHG reduction.

Table S11. Life cycle inventory and GHG emission assessment for the LCA model.

Life Cycle Inventory			LCA: GHG Emissions				
Products							
Hydrocarbon Fuels (Total)	207	kg/hr					
	9854	MJ/hr					
Jet	207	kg/hr					
	9065	MJ/hr					
Naphtha	20	kg/hr					
	790	MJ/hr					
Co-Products			Normalized use (usage unit/MJ)	Carbon intensity	Unit	Data source	Emissions (g CO2 eq/MJ)
BTEX	22.5	kg/hr	0.002287908	-1.16	kg CO2eq/kg	Yadav et al. 2023	-2.65
Resource Consumption			Normalized use (usage unit/MJ)	Carbon intensity	Unit	Data source	Emissions (g CO2 eq/MJ)
Feedstock							
Feedstock (food waste, dry)	2362	kg/hr	0.239740908	-0.745145	kg CO2eq/kg of dry food waste	Consistent with assumptions in Miller et al. 2022	-178.64
Feedstock Moisture	7087	kg/hr					
Feedstock Carbon (% of dry)	0.0%						
Acid Separation							
Iodoform	0.8	kg/hr	7.99056E-05	12.21646704	kg CO2eq/kg	GREET 2021: ZSM-5 (Proxy)	0.98
Ammonium Hydroxide	10.5	kg/hr	0.001070028	1.2807	kg CO2eq/kg	GREET 2021: Ammonium Hydroxide	1.37
Sulfuric acid, 93%	26.0	kg/hr	0.002639056	0.0433831	kg CO2eq/kg	GREET 2021: Sulfuric Acid	0.11
Upgrading							
H2	5.7	kg/hr	0.000573701	11.6651	kg CO2eq/kg	GREET 2021: Compressed gaseous H2 via tube-trailers (central plants)	6.69
Cooling water chemicals	0.0	kg/hr	1.58085E-06				0.00
Water Input	1162	kg/hr	0.117917663	0	kg CO2eq/kg	GREET 2021: Water	0.00
Sulfalone Solvent	4	kg/hr	0.000409029	1.28	kg CO2eq/kg	EcoInvent Database: Dimethyl Sulfoxide (Proxy)	0.52
Catalyst - ZrO2	0.075	kg/hr	7.59634E-06	12.21646704	kg CO2eq/kg	GREET 2021: ZSM-5 (Proxy)	0.09
Catalyst - 3% Pt/Al2O3	0.004	kg/hr	4.51718E-07	12.21646704	kg CO2eq/kg	GREET 2021: ZSM-5 (Proxy)	0.01
Catalyst - HZSM-5	0.027	kg/hr	2.70654E-06	12.21646704	kg CO2eq/kg	GREET 2021: ZSM-5	0.03
Energy Use							
Purchased Natural Gas	0.18	MMBtu/hr	1.81519E-05	73.33	kg CO2eq/MMBtu	GREET 2021: Natural Gas as Stationary Fuels (with emission factor for large industrial boiler)	1.33
Purchased electricity	186	kW	0.018850944	0.4398	kg CO2eq/kWh	GREET 2021: Distributed electricity, U.S. Mix	8.29
Emissions							
Water (H2O)	2007	kg/hr	0.203642635				0
Nitrogen (N2)	36208	kg/hr	3.674350897				0
Oxygen (O2)	10622	kg/hr	1.077898092				0
CO2 (biogenic)	1800	kg/hr	0.182636539	0	kg CO2eq/kg		0.00
CO2 (fossil)	9	kg/hr	0.000945812	1	kg CO2eq/kg		0.95
Waste Streams							
Wastewater (kg/hr BOD)	4	kg/hr	0.000387294	1.6325	kg CO2eq/kg BOD	Shahabadi et al. 2009: Aerobic treatment, no bioga	0.63
Digestate (total)	2038	kg/hr	0.206783594				0.00
Moisture	1111	kg/hr	0.112791051				0.00
Solids	926	kg/hr	0.093992543	0.0946309	kg CO2eq/kg	GREET 2021: AD Residue	8.89
Solids Carbon %	46%		4.71832E-05				0.00
Total							**-151.4**

Table S12. Life cycle inventory and water consumption assessment for the LCA model

Life Cycle Inventory				LCA: Water Consumption			
Products							
Hydrocarbon Fuels (Total)	207	kg/hr					
	9854	MJ/hr					
Jet	207	kg/hr					
	9065	MJ/hr					
Naphtha	20	kg/hr					
	790	MJ/hr					
Co-Products			Normalized use (usage unit/MJ)	Water intensity	Unit	Data source	Water use (L/MJ)
BTEX	22.5	kg/hr	0.002287908	-3.6989	L/kg	GREET 2023: Benzene	-0.008462745
Resource Consumption			Normalized use (usage unit/MJ)				
Feedstock							
Feedstock (food waste, dry)	2362	kg/hr	0.239740908	0	L/kg	GREET 2023: Landfilled food waste	0
Feedstock Moisture	7087	kg/hr					
Feedstock Carbon (% of dry)	0.0%						
Acid Separation							
Iodoform	0.8	kg/hr	7.99056E-05	22.5439429	L/kg	GREET 2023: ZSM-5 (Proxy)	0.001801388
Ammonium Hydroxide	10.5	kg/hr	0.001070028	1.4397417	L/kg	GREET 2023: Ammonium Hydroxide	0.001540564
Sulfuric acid, 93%	26.0	kg/hr	0.002639056	0.3199	L/kg	GREET 2023: Sulfuric Acid	0.000844234
Upgrading							
H2	5.7	kg/hr	0.000573701	21.2448314	L/kg	GREET 2023: Compressed gaseous H2 via tube-trailers (central plants)	0.012188177
Cooling water chemicals	0.0	kg/hr	1.58085E-06				
Water Input	1162	kg/hr	0.117917663	1	L/kg	Freshwater density	0.117917663
Sulfalone Solvent	4	kg/hr	0.000409029	23.9	L/kg	EcoInvent Database: Dimethyl Sulfoxide (Proxy)	0.009775792
Catalyst - ZrO2	0.075	kg/hr	7.59634E-06	22.5439429	L/kg	GREET 2023: ZSM-5 (Proxy)	0.000171251
Catalyst - 3% Pt/Al2O3	0.004	kg/hr	4.51718E-07	22.5439429	L/kg	GREET 2023: ZSM-5 (Proxy)	1.01835E-05
Catalyst - HZSM-5	0.027	kg/hr	2.70654E-06	22.5439429	L/kg	GREET 2023: ZSM-5	6.10161E-05
Energy Use							
Purchased Natural Gas	0.18	MMBtu/hr	1.81519E-05	12.1575696	L/MMBtu	GREET 2021: Natural Gas as Stationary Fuels	0.000220683
Purchased electricity	186	kW	0.018850944	2.3506397	L/kWh	GREET 2021: Natural Gas as Stationary Fuels	0.044311777
Total							**0.18**

Food waste cost (-$50 / $0/wet ton / $76)

Total capital investment (TCI) (-50% / Baseline / +50%)

Food waste CI credit (x1.5 / Baseline / 0)

LCFS credit price (+50% / $133/tonne CO2eq / -50%)

RIN credit price (+50% / $0.81/gal / -50%)

BTEX selling price ($1.36/lb / $0.68/lb / $0.32/lb)

Naphtha selling price (+50% / $2.59/gal / -50%)

$(10.00) $(5.00) $- $5.00 $10.00 $15.00

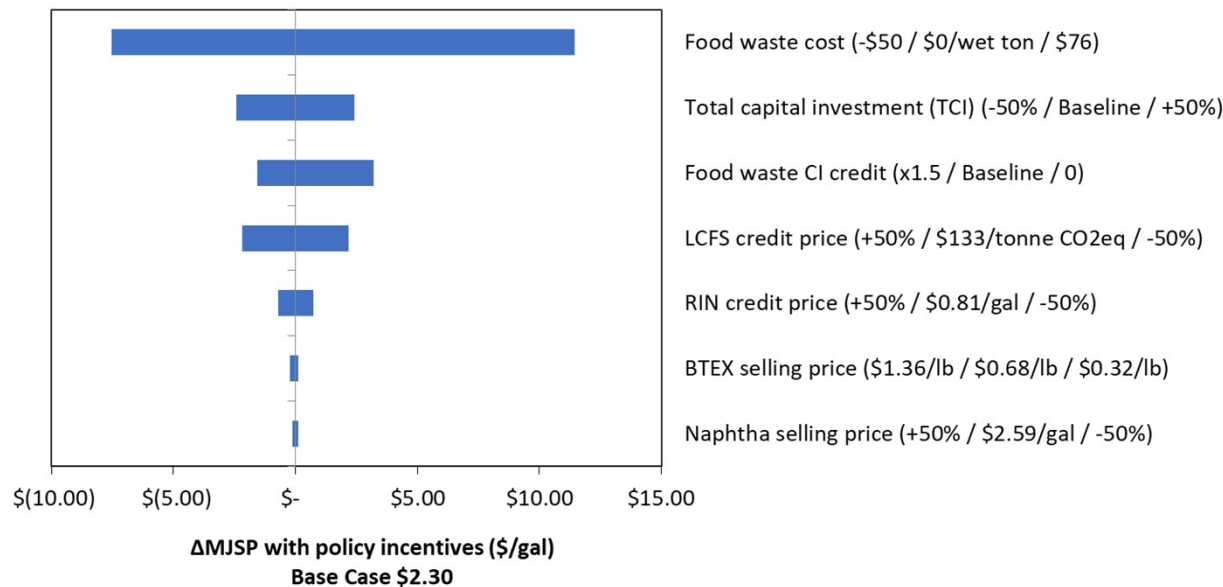ΔMJSP with policy incentives ($/gal)
Base Case $2.30

Figure S10. Tornado plot showing the results of the single-point sensitivity analysis for the TEA model.

Section S4. Wet waste-derived carboxylic acids upgrading research and implementation JUST-R metrics (for TRL 3 research).

The JUST-R metrics are listed in Table S13. Positive metrics (which are sometimes listed as "low" and sometimes listed as "high") are highlighted in green and negative metrics are highlighted in red.

Table S13. JUST-R metrics for VFA upgrading to sustainable aviation fuel and BTEX and related laboratory research.

Metric	Assessment	What could be done differently?	Potential barriers
Anticipation			
Efficiency of resource use	Relatively **high**; the process is predicated on valorizing wet waste that would be otherwise routed to landfills.	Increases in process integration/intensification can maximize the utilization of carbon.	Research in this area would be costly.
Life cycle greenhouse gas emissions	**Low** due to avoidance of GHG emissions from the landfilling of food waste (-151 g CO_2eq/MJ fuel, vs. 90 g CO_2e/MJ for fossil jet)	N/A	N/A
Life cycle water consumption	**Medium**, primarily driven by water requirements for facility cooling towers (0.18 L/MJ, vs. 0.074 L/MJ for fossil jet)	Improved heat integration and use of air cooling when applicable	Alternative cooling methods are outside the scope of this study, but developing these could decrease life-cycle water consumption.
Life cycle air pollution	**Medium**; By arresting AD, we shift from a gaseous energy source (biogas) to a liquid, which results in less fugitive emissions of VOCs; however, the nature of collecting and transporting food waste may result in odors and fugitive VOCs	Careful consideration of food waste supply chain and ensuring proper containment at each stage	Cost and logistics of managing food waste from variety of different sources
Land use	Relatively **low**; the feedstocks for this process need no dedicated land for production and the facilities needed for upgrading are comparable to other biomass upgrading processes.	N/A	N/A
Potential of the research to impact positively/negatively on some social groups	**Medium**; chemical upgrading facility siting often has disproportionate negative impacts on frontline communities, which often comprise higher-than-average levels of underrepresented minorities.	General improvement of chemical plant safety standards and regulations would help to remedy this problem.	Safety and environmental regulation policies are difficult to enact and enforce.
Levels of safety	Relatively **low**; products and reactants are oxygenated and hydrocarbon organic molecules which are not	Adjusting the process to produce no aromatic compounds would remove this risk.	The aromatic compounds made in this process fulfill key roles as polymer precursors and SAF components;

	extraordinarily hazardous or impactful on health. Aromatic compounds are, however, carcinogenic.		research into replacements for these chemicals' end uses would be necessary.
Concentrations of pollutants or toxins	Relatively **low.** As long as the upgrading facility captures light gases produced in the process, all products are benign.	Careful consideration of food waste supply chain and ensuring proper containment at each stage	Cost and logistics of managing food waste from variety of different sources and containment of liquid and gaseous products from catalytic upgrading operations
Reflexivity			
Transparency	**High**. Our methods and decision making are unambiguously laid out in the manuscript.	N/A	N/A
Data availability	**High**. This manuscript is published open access with extensive data availability.	N/A	N/A
Information disclosure	**High**, see above.	N/A	N/A
Accountability level	**High**, see above. Contact information for authors accompanies the manuscript.	N/A	N/A
Capacity to communicate to stakeholders	**Low**. Technical manuscripts are (as an unfortunate byproduct of their design) difficult to process for many potential stakeholders without a specific technical skillset.	We could highlight key findings from our research in more widely available resources (*e.g.*, press releases, blog posts, the NREL website).	Non-technical sources have a limited capacity to highlight findings such as those we present here and general audiences do not have the bandwidth or interest to learn about every advance in clean energy technology.
Percentage of researchers who believe it is important to consider/address issues related to social justice/inclusion in their research methodology	**High**, our research team believes in these principles.	N/A	N/A
Inclusion			
Job opportunities	**Medium**. Implementing wet waste upgrading to SAF and chemical precursors would generate job opportunities across the upgrading pathway (feedstock collection/handling, biological and thermochemical upgrading) for workers with a variety of levels of educational attainment.	A targeted study of this economic tradeoff is beyond the scope of this work but would reveal more quantitative insights into this tradeoff.	Such a targeted study would require a separate and substantial source of funding.

	However, the transition away from petrofuels and petrochemicals will also eliminate established jobs in these sectors.		
Education	**Medium**. Interns and early-career researchers have been involved in this work, but more efforts to reach out to youth populations could be undertaken.	Our research team could develop a general population- and youth-friendly methodology for presenting our work.	This is a non-negligibly difficult task.
Institutional representation	**Low**. Citizens who would interact with this technology (*e.g.*, residents of possible frontline communities for wet waste collection and upgrading) have not been engaged in this research.	Our research team could perform more outreach in these communities.	This would be a complicated and time-consuming task with potentially low buy-in or interest from stakeholders, as this work is still far from implementation.
Level of ability of the research problem to address an access problem of a disadvantaged social group	**Medium**. Decarbonizing aviation fuel and chemicals would not preferentially benefit disadvantaged social groups. However, members of disadvantaged social groups are disproportionately harmed by emission of hazardous chemicals from unremediated wet waste such as concentrated animal feeding operations.[15,16] Bringing these wet wastes into an upgrading supply chain would mitigate the harm to these populations.	This situation is a structural feature of the problem being solved.	N/A
Compatibility with culture	**Medium**. Implementation of this wet waste upgrading strategy would ease stress on frontline communities (see above), but other effects are negligible.	This situation is a structural feature of the problem being solved.	N/A
Hidden process costs			
Estimated cost of managing waste generated by the research	**Low**. Organic and aqueous liquid waste (~0.1s-1s L), inert salt and catalyst waste (0.1s kg), and precious metal catalyst waste (~1s g) are mitigated via	This setup is close to optimal for low TRL research.	N/A

	conventional remediation protocols. Volumes generated in this research are not large enough to significantly contribute the overall volumes generated at the National Renewable Energy Laboratory.		
Estimated cost of energy consumed during the research	**Medium**. Resistive reactor heating, GC/MS operation, and ventilation operation are relatively energy consuming.	Reactor heating, GC/MS instruments, and ventilation are run over all hours, so running at times of high grid stress is unavoidable apart from designing more energy efficient instruments.	Designing more energy efficient reactor heaters, GC/MS instruments, and ventilation systems are outside the scope of our research.
Projected cost savings from operating the new technology vs. competing technologies	**Medium.** The cost of our SAF to consumers will be similar to that of fossil jet.	Further improvements in our technology (increased selectivity, lower energy use) can cause a decrease in price.	Improving the technology will take further R&D. Clean fuel subsidies are necessary to keep the price in this range, or else the assessment value would be high (unfavorable).
Breadth of pre-existing knowledge review			
Number of social science papers reviewed	**Medium**. Authors are familiar with social science literature reviewing adverse impacts of wet waste on frontline communities,[15,16] but not with literature concerning other crucial applications such as localized impacts of biochemical plants.	Researchers could read more into literature concerning impacts of other important components of the process discussed in this manuscript.	The only roadblock here is researcher time investment.
Diversity of authors of scientific papers reviewed	**Low.** Out of all publications cited in the main body of this work, only six are written by non-male first authors, only three come from institutions in locations other than the United States or Europe, and only one is written by a first author belonging to a minority group historically underrepresented in STEM.	Authors could attempt to selectively search for relevant papers in the field written by diverse authors. However, this solution is incomplete; it is a symptom of the broader lack of diversity in STEM.	Author time could be invested in such a selective search, but the problem will be best solved by increasing the diversity of researchers in the field.
Number of nonacademic sources reviewed	**Low**. The authors are not aware of nonacademic sources that are relevant	Researchers could conduct an extensive review of blogs, local	The only roadblock here is researcher time investment.

	to this low-TRL research.	news sources, and books pertinent to this research.	
Distribution of research results			
Proportion of results published open access	**High**. This paper is published open access.	N/A	N/A
Number of nonacademic reports of results	**Low**. This report is the first published about these specific results.	Authors could work to promote this work via non-academic outlets (social media, etc.) to broaden interest from non-academic parties.	Authors will do this.
Number of nonacademic oral presentation of results	**Medium**. The lead author (JHM) presented work on wet waste upgrading to SAF at a statewide recycling conference geared toward community activists.	Authors could continue to seek out such opportunities.	Authors will do this.
Diversity of audience reached	**Low**. This report is the first published about these specific results and academic journals, even if open access, are not read broadly outside of highly specialized communities.	Authors could work to promote this work via non-academic outlets (social media, etc.) to broaden interest from non-academic parties.	Authors will do this.
Diversity of team members credited for and publicly presenting work	**Medium**. The research team contains women and members of underrepresented communities, but the lead/corresponding author responsible for presenting this work is a cisgender white male.	The research team can work to ensure that a diverse team continues to work on this project and that leadership positions are distributed equitably.	Researchers will do this.
Distribution of hazard exposure during the research life cycle			
Hazard level of extracting or synthesizing material inputs	**Medium**. All feedstocks are germane waste products, and major catalysts (H/ZSM-5, ZrO_2) are inexpensive and relatively nonhazardous to collect. Precious metal catalyst components used in this work (Pt, Pd) are more hazardous to produce and are envisioned to be substituted with metals less hazardous to extract (*e.g.*, Ni, Mo) after scale-up.	Lab-scale hydrodeoxygenation could be undertaken with non-precious metal catalysts.	These non-precious metal catalysts must be operated with a sulfiding agent co-feed, which presents localized safety hazards.
Hazard level of laboratory processes	**Low**. All systems used for conversion are designed to minimize risk to researchers.	N/A	N/A

Hazard level of managing waste	**Low**. All systems used for waste management are designed to minimize risk to workers.	N/A	N/A
Extent to which hazards would increase at industrial scale	**Medium**. All steps of this process are similar to other currently implemented industrial processes.	Currently implemented industrial processes could be scrutinized and improved further for hazard avoidance.	These activities would likely require legislation to be passed that increases government oversight and regulations.
Identification of set vs. flexible parameters			
Number of alternatives explored to waste-intensive processes	**None**.	Experimental protocols could be optimized to minimize solvent use, reactor uptime, etc.	Experiments are constantly changing, so optimizing them would be challenging.
Number of alternatives explored to energy-intensive processes	**None**.	Experimental protocols could be optimized to minimize solvent use, reactor uptime, etc.	Experiments are constantly changing, so optimizing them would be challenging.
Number of alternatives explored to hazardous or unethically sourced materials	**None**.	Experimental protocols could be optimized to minimize solvent use, reactor uptime, etc.	Experiments are constantly changing, so optimizing them would be challenging.
Number of environmental parameters tested	**None**.	Researchers could prioritize using more environmentally-friendly solvents for instrument cleaning and upkeep.	Ordering these chemicals in bulk may be complicated, as they are not integrated with the overall lab solvent infrastructure.
Number of nontechnological solutions explored to solve key problems within the research	**None**.	Researchers could encourage the public to decrease use of aviation and materials derived from aromatic molecules.	Most of the general population (many of these authors included) is unprepared to implement these types of substantial lifestyle changes.

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