Supporting Information

for

Characterizing the Opportunity Space for Sustainable Hydrothermal Valorization of Wet Organic Wastes

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This Supporting Information contains 32 pages, 14 tables, and 7 figures.

S1. Feedstock characterization

Organic wastes serving as feedstocks for the HTL-based treatment train were characterized based on their moisture content, ash content, and biochemical compositions (lipids, proteins, carbohydrates) (**Table S1**). Based on these assumptions, their elemental compositions were also estimated based on a multi-component linear relationship (**Table S2**). Specifically, carbon, hydrogen, and nitrogen content of lipids ($C_8H_{16}O$), proteins ($C_{16}H_{24}O_5N_4$), and carbohydrates $(CH₂O)$ were estimated based on their empirical chemical formula.¹ Phosphorus was estimated based on reported nitrogen to phosphorus ratio for different feedstocks (**Table S1**). Oxygen was estimated based on mass balance as $1 - C$ (dry weight, dw%) – H (dw%) – N (dw%) – P (dw%) $-$ ash (dw%).

Organic Waste	Moisture	Ash	Biochemical compositions [ash-free dry weight%]	P to N mass	Ref.		
	[%]	[dry weight%]	Lipids	Proteins	Carbohydrates	ratio	
Sludge	$60 - 80\%$	$17.4 - 41.4%$	$8 - 30.8%$	$38 - 51%$		19.4-55.6%	$2 - 6$
Fats, oils, and greases (FOG)	$10 - 60%$	1.49-2.24%	$91.2 - 100\%$	$0 - 1.23%$		$0 - 3.5%$	$7 - 10$
Food waste	68-80%	$2.5 - 12.6%$	$13 - 30%$	$15 - 25%$	$100\% -$ lipids $\%$ $-$ proteins%	11.5-28.6%	5.6.10 -12
Green waste	$5.2 - 69%$	$1.2 - 48.3%$	$1.04 - 2.59%$	$1.6 - 8.2%$		18.7-22.9%	$13 - 15$
Animal manure	17.4-79.8%	$13.8 - 43%$	$3.77 - 24.7%$	$14.3 - 26.4%$		25.3-38.0%	3,4,16

Table S1. Biochemical compositions of different organic wastes.

a Uniform distribution.

S2. System design

1. Design basis

The design for HTL-based treatment system was executed using newly released QSDsan^{17,18} (using 'pfas' branch updated as of October 28, 2023), a comprehensive modeling platform for quantitative sustainable design of sanitation and resource recovery systems. All the units were coded using python 3.9 and can be publicly accessed through GitHub-Quantitative Sustainable Design (QSD) Group-repositories.¹⁸ The proposed system configuration was based on a 2014 PNNL report,¹⁹ with the addition of struvite precipitation and membrane distillation for nutrient recovery. Detailed unit design assumptions and methods can be found in the following sections. Units not discussed below (e.g., heat exchanger, flash vessel, distillation column) were inherited from previous work in QSDsan and BioSTEAM^{20,21} (using 'gsdsan' branch updated as of October 28, 2023).

2. Detailed design assumptions and methods

i. Hydrothermal liquefaction (HTL)

HTL converted wet biomass into biocrude, hydrochar, an aqueous phase, and off-gas under subcritical temperatures (250 to 350 °C) and high pressure (3050 psia). We used a revised multicomponent additivity (MCA) model^{22,23} to estimate the yields and elemental compositions of each HTL product (**Table S3**). All calculations were done on an ash free dry weight (afdw) basis. Except for lipid-to-biocrude (0.846) which followed a triangular distribution, other parameters with uncertainties were assigned normal distributions. All ash content from HTL feedstocks were assumed to be partitioned into the aqueous phase (consistent with Leow et al.²³). The gas phase was >90% $CO₂$ with a small amount of $CH₄$ and $C₂H₆$. The gas compositions were based on simulations from Jones et al.¹⁹ Biocrude moisture content was 5.6%, the same as our reference model.¹⁹

Table S3. Revised MCA model parameters.

Elemental distributions in HTL oil and solid phases were calculated based on MCA model (**Table S4**), with AOSc (average oxidation state) calculated using the equation in Li et al.²² Carbon in the gas phase was calculated based on estimated gas compositions. Nitrogen was assumed to partition to the biocrude and aqueous phases. $2^{3,24}$ 86% (84 to 88%) of phosphorus was assumed to be in hydrochar after the HTL reaction in the form of inorganic phosphate.^{24,25} The remaining phosphorus was assumed to be in the aqueous phase. The MCA model can also be used to estimate the TOC and TN concentrations (in mg $\cdot L^{-1}$) in the aqueous phase product, but in this study elements in the aqueous phase were calculated based on mass balance closure to accommodate uncertainties associated with the aqueous phase volume. The MCA was validated on wastewater sludge and animal manure in Li et al.²² Validation for food waste, FOG, and green waste (limited to the biocrude yield) were included in **Table S5**. The auxiliary units for HTL include

knockout drums for gas separation, a solid filter for hydrochar recovery, and a gravimetric oil/water separator to vent gas and separate biocrude and aqueous phase by gravity, and knockout drums to remove any liquid from the off-gas.

Elemental Composition	Input	Slope	Intercept
Biocrude-C	AOSc	$-8.37 (\pm 1.84)$	68.6 (\pm 0.72)
Biocrude-N	Protein [dw%]	$0.133 (\pm 0.010)$	
Biocrude-H	AOSc	$-2.61 (\pm 0.69)$	$8.20 (\pm 0.27)$
Hydrochar-C ^a	Carbohydrate [dw%]	$1.75 (\pm 0.24)$	_

Table S4. MCA model parameters for elemental composition of biocrude.

^a The smaller value between the calculated result and 0.65 was used.

Table S5. Experimental data (from literature) and MCA predicted biocrude yields (for food waste, FOG, and green waste).

As the feedstocks for HTL reactor at low temperatures have very high viscosity (0.002 to 0.065 m²·s⁻¹),³² the heat exchanger for HTL feedstock heating is typically overdesigned to overcome the potential fouling issue. In our design, we enforced the total heat transfer efficiency of HTL heat exchanger to 3 to 4 BTU·hr⁻¹·ft⁻²·F⁻¹ (0.0170 to 0.0227 kW·m⁻²·K), which was an order of magnitude lower than the heat transfer efficiency of low-viscosity feedstock (26 to 274 BTU·hr⁻¹·ft⁻²·F⁻¹).³² The HTL heat exchanger design process included the following steps:²¹

1. Calculated the log-mean temperature difference (*LMTD*) of an ideal counterflow or cocurrent heat exchanger using **Eq. S1** to **Eq. S5**.

$$
dTF_1 = T_{h,l} - T_{c,o} \tag{S1}
$$

$$
dTF_2 = T_{h,o} - T_{c,i} \tag{S2}
$$

$$
dTF_{2,1} = dTF_2 - dTF_1 \tag{S3}
$$

where $T_{h,l}$, $T_{c,o}$, $T_{h,o}$, and $T_{c,i}$ represented inlet temperature of hot fluid [K], outlet temperature of cold fluid [K], outlet temperature of hot fluid [K], and inlet temperature of cold fluid [K], respectively. If the absolute value of $dTF_{2,1}$ was less than 10⁻⁸:

$$
LMTD = dTF_1 \tag{S4}
$$

If not:

$$
LMTD = \frac{dTF_{2,1}}{\ln \frac{dTF_2}{dTF_1}}
$$
(S5)

2. Calculated the heat transfer area (A) of HX tubes using **Eq. 6**.

$$
A = \frac{Q}{U \cdot LMTD \cdot ft}
$$
 (S6)

where *Q* was the heating duty (including environmental losses) [kJ·hr−1] of the heat exchanger, *U* was the enforced total heat transfer efficiency [kW·m⁻²·K⁻¹], and *ft* was the *LMTD* correction factor and can be calculated based on equations in Fahkeri et al. If *A* was less than 150 ft², we assumed the heat exchanger type to be double pipe. If not, we assumed the heat exchanger type to be floating head.

3. Calculated the purchase cost [2013\$] of the HTL heat exchanger based on the type using **Eq. 7** or **Eq. 8** and converted the cost to 2020\$.

purchase cost (double pipe) = $e^{7.2718+0.16 \cdot \ln A}$ (S7)

purchase cost (floating head) = $e^{12.0310-0.8709 \cdot \ln A + 0.09005 \cdot (\ln A)^2}$ (S8)

ii. Catalytic hydrothermal gasification (CHG)

HTL aqueous phase had very high COD content, therefore, cannot be discharged directly. CHG was used in our system after struvite precipitation (discussed below) to valorize COD to fuel gases. Heterogeneous catalyst 7.8% Ru/C (7.8% w/w ruthenium on a carbon support) was used in CHG.¹⁹ About 56.55% of carbon was gasified into CH₄, C₂H₆, C₃H₈, and CO₂, with the ratio (**Table S6**) referred to by Jones et al.¹⁹ CHG products were then passed to a flash vessel to separate gas based on vapor-liquid-equilibrium (VLE). Gas components were sent to a combined heat and power (CHP) unit and can provide energy and electricity for the system.³⁴ The rest of carbon and nitrogen were assumed to be in the forms of HCO $_3^-$ and NH $_4^{\ast}$ in CHG effluent.¹⁹

Product	CHG ^a	hydrotreating	hydrocracking
H ₂	0.0001		
CO ₂	0.432		0.0388
Methane	0.527	0.0228	0.0063
Ethane	0.011	0.0292	
Propane	0.030	0.0165	
Butane		0.0087	
Butane, 2-methyl-		0.0041	
Pentane		0.0068	
Pentane, 2-methyl-		0.0041	
Hexane		0.0041	0.0116
Hexane, 2-methyl-		0.0041	
Heptane		0.0041	0.1202
Cyclohexane, methyl-		0.0102	
Piperidine		0.0041	
Toluene		0.0102	
Heptane, 3-methyl-		0.0102	

Table S6. CHG, hydrotreating, and hydrocracking products (values shown in w/w).

a Not including H₂O and soluble components.

iii. Hydrotreating

Biocrude from HTL needed to be further upgraded to meet the market requirement. Widely used hydrotreating followed by hydrocracking (next section) was selected for HTL biocrude refinement. Major assumptions made for hydrotreating were:

- 1. The H_2 amount reacted was assumed to be fixed at 4.6 wt% of biocrude, the same as previous work.²³ However, to maintain a H_2 headspace and ensure complete reaction, 3 times the reacted H_2 amount was fed.¹⁹
- 2. 87.5 wt% of biocrude and reacted H_2 were converted to hydrocarbon with CoMo/alumina (cobalt molybdenum on an alumina support) as the catalyst.¹⁹
- 3. The hydrotreating products were scaled from the reference. The percentages of each product can be found in **Table S6**.
- 4. One flash vessel and three distillation columns in series were used to separate hydrotreating products into aqueous, fuel gas, naphtha, diesel, and heavy oil. The aqueous phase was discharged and managed at a water resource recovery facility (WRRF; a.k.a. wastewater treatment plant, WWTP), fuel gases were burnt in the CHP system, naphtha and diesel were cooled down before storage, and heavy oil was further cracked in a hydrocracking unit. Flash vessel and distillation columns were inherited from BioSTEAM.

iv. Hydrocracking

Hydrocracking further broke down heavy oil from hydrotreating to naphtha and gasoline. Major assumptions for hydrocracking design included:

- 1. The amount of H_2 reacted was assumed to be fixed at 1.1 wt% of heavy oil, the same as previous work.²³ However, to maintain a H_2 headspace and ensure complete reaction, 5.6 times the amount of reacted H_2 was fed.¹⁹
- 2. 100 wt% of heavy oil and reacted H_2 was converted to hydrocarbon with CoMo/alumina as the catalyst.¹⁹
- 3. The hydrocracking products were scaled from the reference. The percentages of each product can be found in **Table S6**.
- 4. One flash vessel and one distillation column were used to separate hydrocracking products into fuel gas, naphtha, and diesel. Fuel gas was burnt in the CHP system; naphtha and diesel were cooled down before storage.

v. Phosphorus recovery

86% of phosphorus stayed in HTL produced hydrochar and could be extracted and recovered as fertilizers.^{24,25} Therefore, an acid extraction followed by struvite precipitation was proposed for phosphorus recovery. According to proposed system flow, an average of 70% (49.9% to 90.2%) phosphorus^{24,25} in hydrochar was extracted by acid (0.5 M H_2SO_4 , 1:10 g·mL⁻¹). Then, phosphorus-rich extractant was mixed with the NH₄⁺-rich HTL aqueous stream for struvite precipitation, supplemented with MgCl₂ (molar ratio Mg:PO₄^{3–} = 1.5:1 to 4:1) and NH₄Cl (if needed, to ensure excess amount of N). MgO was also added to maintain a pH of around 9.5^{35} The reported K_{sp} of struvite in the literature is usually smaller than 10⁻¹⁰.³⁶ Therefore, instead of using a kinetic model (which always predicted ~100% phosphorus precipitation), we estimated phosphorus recovery based on published experimental data and assumed the baseline struvite precipitation recover 82.8% of phosphorus.²⁵

vi. Nitrogen recovery

Part of the nitrogen in the HTL aqueous phase was recovered with phosphorus during struvite precipitation. The rest of the nitrogen (both organic and inorganic) was converted to NH₄⁺ during CHG. The high concentration of NH₄⁺ precluded the possibility of direct discharge of CHG effluent. A membrane distillation unit was therefore modeled to recover NH_4^+ as ammonium sulfate. The driving force of the membrane distillation was the vapor pressure difference of $NH₃$ across a hydrophobic membrane generated due to different temperature and pH between the feed side and permeate side. 0.5 M H₂SO₄ was used to produce ammonium sulfate in the permeate side. The flux of ammonia across the membrane was calculated using the equation below: 37

$$
J_{NH_3,f} = k_f C_{NH_3,f} ln(\frac{X_{NH_3,f,m} - X_{NH_3,p}}{X_{NH_3,f} - X_{NH_3,p}})
$$
(S9)

kf was the feed side mass transfer coefficient and can be calculated using **Eq. S10**. ³⁸ *CNH3* was the concentration of NH₃ in the feed and can be calculated as a function of feed pH value. $X_{NH3,f,m}$, *XNH3,f*, and *XNH3,p* were NH3 molar fractions in membrane, feed, and permeate, respectively. *XNH3,p* was approximated as 0 due to low pH in the permeate. $X_{NH3,f,m}$ and $X_{NH3,f}$ were calculated using the established VLE relationship in BioSTEAM.

$$
\frac{1}{K_a} = \frac{1}{k_f} + \frac{1}{Hk_m} \left(1 + \frac{k_b}{[OH]} \right)
$$
 (S10)

Ka was the overall mass transfer coefficient and was estimated based on published experimental data.38 *H* was dimensionless Henry's law constant and was calculated using **Eq. S11**. ³⁹ *km* represented the membrane mass transfer coefficient and was calculated using **Eq. S12.**³⁸ k_b was the base dissociation constant of NH₃ and can be calculated by Eq. S13.

$$
H = \frac{H'}{RT}
$$
 (S11)

H' is the Henry's law constant with dimension for NH₃ (1.63 Pa·m³·mol⁻¹). *R* is the ideal gas constant (8.3145 Pa·m³·mol·K⁻¹) and *T* is the influent aqueous temperature (333.15 K).

$$
k_m = \frac{D_m \varepsilon}{r \delta} \tag{S12}
$$

ε, τ, and *δ* were membrane porosity, tortuosity, and thickness, respectively. *Dm* was the molecular diffusivity of ammonia in air. 40

$$
k_b = \frac{k_w}{k_a} \tag{S13}
$$

kw was the water dissociation equilibrium constant. *ka* was the acid dissociation constant of NH4 ⁺ at 333.15 K and can be adjusted based on the van't Hoff equation (**Eq. S14)**.

$$
\ln\left(\frac{k_a}{k_{a,0}}\right) = \frac{\Delta H^0}{R} \left(\frac{1}{T_0} - \frac{1}{T}\right)
$$
\n(S14)

*K*_{a,0} was the acid dissociation constant of NH₄⁺ at *T*₀ (298 K). ∆H⁰ was the standard enthalpy of the NH₄⁺ dissociation reaction (52.22 kJ·mol^{−1}) at T_o .

The baseline values and distribution of other parameters included in this section can be found in **Table S11**.

vii. Unit designs

The designs (dimensions and material usage) of HTL, CHG, hydrotreating, hydrocracking, acid extraction (AcidEx), and struvite precipitation (StruPre) were done using BioSTEAM design tools. Detailed parameters can be found in **Table S7**. The flash vessel and distillation column were inherited from BioSTEAM without changes.

Parameter	HTL	CHG		hydrotreating hydrocracking AcidEx StruPre		
Temperature (T) [°C]	351	349	402	451	25	25
Pressure (P) [MPa]	21.0	21.2	10.5	7.0	0.1	0.1
# of reactors (N) [-]	4	6	1	1	$\overline{2}$	2
Single reactor volume [m ³]	3.65	2.37	11.4	6.11	10	20
Length [m]	152	2.3	3.9	3.1	3.7	4.7
Inner diameter [m]	0.18	1.15	1.94	1.57	1.85	2.33
Wall thickness [m]	0.03	0.18	0.14	0.11	0.01	0.01
Tau ^a [h]	0.25	0.33	0.5	5	$\overline{2}$	
Type	pressure vessel (PV)	PV	PV	PV	storage tank	storage tank
Material	stainless steel (SS) 316	SS 316	SS 316	SS 316	SS 304	carbon steel
Vessel type	Horizontal	vertical	vertical	vertical	vertical	vertical
WHSV ^b $[g \cdot g^{-1} \cdot h^{-1}]$		3.56	0.625	0.625		

Table S7. Design parameters for unit operations in the HTL-based treatment train (100 dry tonne·day⁻¹ capacity).

^a Retention time.

b Weight hourly space velocity.

S3. Mass and energy balance

Using QSDsan, the influent and effluent streams of each unit were automatically simulated to determine the mass and energy flows, enabling mass balances for key elements (i.e., carbon, nitrogen, and phosphorus). Energy balances considered heating/cooling of units, thermal losses, and streams' chemical energy (measured as higher heating values, HHVs). For streams consisting of defined chemicals (e.g., diesel consisting of chemicals listed in **Table S6**), we used BioSTEAM for HHV calculations. For streams that did not require full characterization or for which full composition details were unknown (e.g., organic wastes), we estimated their elemental composition and calculated their HHV using the Dulong equation:⁴¹

HHV (MJ·kg⁻¹) = 0.338 × C% + 1.428 × (H% – 0.125 × O%)
$$
(S15)
$$

where C%, H%, and O% represent dry weight% of carbon, hydrogen, and oxygen, respectively.

S4. Techno-economic analysis (TEA)

The capital cost and operation and maintenance cost calculations were automated using existing algorithms in QSDsan.⁴² The capital costs (purchase cost and total installed cost, TIC) for key equipment in the HTL-based system was listed in **Table S8**. Information for operation and maintenance cost estimation (e.g., chemical prices, labor costs) were included in **Table S9**.

Purchase cost [\$]	Total Installed cost [\$]
HTL	
92,400	159,000
875,000	1,480,000
1,800,000	3,540,000
605,000	1,500,000
432,000	820,000
CHG	
98,000	169,000
791,000	1,660,000
35,400	70,800
1,460,000	3,600,000
414,000	1,020,000
271,000	667,000
CHP ^a	
N/A ^b	12,400,000
N/A	4,860,000
N/A	5,160,000
N/A	1,790,000
	Hydrotreating & Hydrocracking

Table S8. Capital costs for key equipment in an HTL-based system (100 dry tonne·day−1 capacity).

^a The cost of CHP was allocated to different based on percentage of energy provided (HTL: 39.2%, CHG: 41.7%, hydrotreating & hydrocracking: 14.4%, exported as electricity: 4.8%).

^b Only the installed cost of CHP was calculated using equations from Shoener et al.³⁴ and Havukainen et al.43

Integrated TEA-LCA were performed based on *n*th plant assumptions, which exclude any cost and environmental impacts due to technological immaturity (consistent with the standards of practice in bioenergy assessments^{6,19}). We used discounted cash flow rate of return analyses to calculate the waste management cost and (separately) the minimum diesel selling price (MDSP). Specifically, the initial capital costs (CAPEX) were distributed over the plant's lifetime with a discount rate to account for the time value of money. Operation and maintenance (O&M) cost were determined by the QSDsan cost algorithms with assumptions in **Table S9**. For auxiliary units (e.g., knockout drum, sulfur guard), costs were scaled using parameters provided in Jones et al.19 Detailed TEA procedures can be found in the QSDsan tutorial paper.¹⁷

Table S9. TEA baseline assumptions.

S5. Life cycle assessment (LCA)

Unit environmental impacts of the HTL-based system were estimated based on the raw material requirements and emissions during construction and operation of the facility. We report environmental impacts across nine impact categories from the U.S. EPA's Tool for the Reduction and Assessment of Chemicals and Other Environmental Impacts (TRACI).⁴⁴ Life cycle inventory data were gathered from the Ecoinvent v3.8 database.⁴⁵ A summary of the unit impacts for raw materials, ancillary inputs, and unit processes are summarized below. The nine impact categories include global warming potential (GWP; a.k.a. carbon intensity, CI), acidification (ACD), ecotoxicity (ECO), eutrophication (EUT), ozone depletion (OZD), photochemical oxidation (PHO), carcinogenics (CAR), noncarcinogenics (NCA), and respiratory effects (RES). The values of unit impacts for each individual construction item, material, and energy source are listed in **Table S10**. A detailed description of LCA algorithms was provided in Li et al.17

Raw Materials, Ancillary		GWP	ACD	ECO	EUT	OZD	PHO	CAR	NCA	RES
Inputs, Unit Processes	Unit	kg CO ₂ -eq	$[H^*]$ -eq	kg 2,4-D-eq	kg N-eq	kg CFC-11-eq	$kg NOx-eq$	kg benzene-eq	kg toluene-eg	$kgPM2.5 - eq$
Furnace	kg	1.26	0.45675	2.5042	0.00047234	7.1820E-08	0.0036727	0.044932	49.582	0.0026779
Concrete	kg	0.11295	0.019506	0.048836	2.4132E-05	$6.02E - 09$	0.0003157	0.00022	1.2785	0.00007732
Compressor (4kW)	ea	670.18	532.58	3736.8	0.2647	$4.55E - 05$	2.5206	90.241	79229	2.891
Compressor (300kW)	ea	12540	8314.4	57484	4.2713	0.00077645	43.493	1361.3	1215800	47.312
Stainless steel	kg	4.8562	1.2979	7.2036	0.00083218	1.96E-07	0.012186	0.13854	164.73	0.016851
Carbon steel	kg	2.0028	0.40517	2.0272	0.00060429	$8.76E - 08$	0.0048205	0.010698	25.211	0.0031905
Reinforcing steel	kg	2.169	0.41317	1.7266	0.00048311	$1.02E - 07$	0.0053051	0.007312	24.747	0.0032199
RO membrane	m ²	2.2663	0.53533	0.90848	0.0028322	$2.55E - 07$	0.0089068	0.034791	31.8	0.0028778
H ₂ SO ₄	kg	0.008206	0.019679	0.069909	$4.05E - 06$	$8.94E - 10$	$5.04E - 05$	$1.74E - 03$	1.6824	$9.41E - 05$
MgCl ₂	kg	2.8779	0.77016	0.97878	0.00039767	4.94E-08	0.0072306	0.005094	8.6916	0.004385
H ₂	kg	1.5624	0.81014	0.42747	0.0029415	$1.80E - 06$	0.0052545	0.002627	8.5687	0.0036698
MgO	kg	1.1606	0.12584	2.7949	0.00063607	$1.54E - 08$	0.0017137	0.018607	461.54	0.0008755
NaOH	kg	1.2514	0.33656	0.77272	0.00032908	7.89E-07	0.0033971	0.007004	13.228	0.0024543
NH ₄ Cl	kg	1.525	0.34682	0.90305	0.0047381	$9.22E - 08$	0.0030017	0.010029	14.85	0.0018387
Struvite	kg	0.42085	0.12283	0.26961	0.00017495	2.2955E-08	0.0010441	0.002983	4.4965	0.0006176

Table S10. Unit impacts of raw materials, ancillary inputs, and unit processes.

S6. Uncertainty analysis

The criteria for the selection of uncertainty distributions followed guidance by Li et al.⁴⁶ with modification.

- Criterion 1. For parameters where the distributions can be found in literature (e.g., MCA model coefficients), we used the same distributions as the literature.
- Criterion 2. For parameters where only the ranges can be found in literature (e.g., sludge moisture), we chose a uniform distribution with the minimum and maximum limits as the lower and upper bounds of the distribution and the average value of the minimum and maximum limits as the baseline.
- Criterion 3. For parameters where only a single value can be found in the literature and is based on empirical formulae (e.g., elemental coefficients in **Table S2**), this value was assigned as the baseline and uniform distributions were set from 90% to 110% of the baseline value.
- Criterion 4. For parameters with no known distribution in the literature:
	- Criterion 4.1. If more than 20 data points were found in the literature, we selected triangular distributions and used $5th$, 50th, and 95th percentiles from the literature values as the minimum, most probable, and maximum values.
	- Criterion 4.2. If only 5 to 20 data points were found in the literature, we selected triangular distributions and used minimum, average, and maximum of the literature value as the minimum, most probable, and maximum values.
	- Criterion 4.3. If less than 5 data points can be found in the literature, we selected uniform distributions and used 80%, 100%, and 120% of the average value as lower bound, baseline, and upper bounds.

A complete list of distributions for each parameter used in the model can be found below (**Table S11**).

Table S11. List of parameters included in the uncertainty analyses. TP = technological parameters; DV = decision variables; CP = contextual parameters.

^a Explanation of parameter names are available online.¹⁸

 $^{\rm b}$ Only for when wastewater sludge as the feedstock and water resource recovery facility (WRRF) size as the independent variable.

S7. Supplemental results

Figure S1. Pinch analysis for the heat transfers in the heat exchanger network (when the feedstock was wastewater sludge). Red horizontal lines represent streams that were heated, and blue horizontal lines represent streams that were cooled. Vertical lines bound by black outlined circles indicate heat transfer across process streams, with the amount of energy transfer marked in the middle squares. Red and blue outlined circles on horizontal lines indicate additional heating or cooling was needed for the streams to reach the final temperature. Units associated with the streams were (HTL) 1, 9; (CHG) 2, 3, 10; (hydrotreating & hydrocracking) 4, 5, 6, 7, 8, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20.

Figure S2. (A) Minimum diesel selling price (MDSP) and (B) carbon intensity (CI) of HTL-based resource recovery systems for fats, oils, and greases (FOG) as a commodity. Middle lines and the band represent 50th and 5th/95th percentiles of 1,000 Monte Carlo simulations. Purple band/line indicate the market price of diesel (data from 2018 to 2022; 2.37 to 5.81 \$·gal⁻¹⁴⁷) in (A) and petroleum diesel carbon intensity (101 kg CO₂ eq·MMBTU^{−1 48}) in (B). Vertical dashed lines indicate the break-even point where the 95th percentile of simulated HTL-based systems is equivalent to the upper level of the current diesel price or carbon intensity. Arrows are oriented to highlight the x-axis values that represent the opportunity space for the HTL-based system.

Figure S3. Breakdowns of categorized (A) cost and (B) CI to each area of the hydrothermal sludge management system. The left stacked bar in each figure is associated with the left y-axis while the middle and right stacked bars are associated with the right y-axis, as indicated by the black arrows. TIC represents the total installed cost. *Utility* in both figures includes heating, cooling, and electricity. The sum of each column is listed above the figures. A tabulated breakdown of data can be accessed online.18

Figure S4. Breakdowns of categorized (A) cost and (B) CI to each area of the hydrothermal wastewater sludge management system (after removing the acid extraction from the original design, Alternative 1). The left stacked bar in each figure is associated with the left y-axis while the middle and right stacked bars are associated with the right y-axis, as indicated by the black arrows. TIC represents the total installed cost. *Utility* in both figures includes heating, cooling, and electricity. The sum of each column is listed above the figures. A tabulated breakdown of data can be accessed online.18

Figure S5. Breakdowns of categorized (A) cost and (B) CI to each area of the hydrothermal wastewater sludge management system (after adding a PSA unit to the original design, Alternative 2). The left stacked bar in each figure is associated with the left y-axis while the middle and right stacked bars are associated with the right y-axis, as indicated by the black arrows. TIC represents the total installed cost. *Utility* in both figures includes heating, cooling, and electricity. The sum of each column is listed above the figures. A tabulated breakdown of data can be accessed online.18

Figure S6. The effects of the water resource recovery facility (WRRF) size on (A) hydrothermal wastewater sludge management cost, (B) hydrothermal wastewater sludge management carbon intensity (CI), (C) MDSP, and (D) biofuel production CI. Figures (A) and (B) are from the waste management perspective, whereas Figures (C) and (D) are from the renewable diesel production perspective. Dotted, dashed, and the middle lines represented $5th/95th$, $25th/75th$, and $50th$ percentiles from 1,000 Monte Carlo simulations. The vertical straight lines indicate the baseline WRRF size (100 MGD) used in this study. Gray shaded areas in each figure represent (A) current wastewater sludge management cost, (B) current wastewater sludge management CI (only covers part of the current value [−245 to 2200 kg CO2 eq·tonne⁻¹] for figure readability), (C) commercial diesel price range, and (D) petroleum diesel production CI.

Figure S7. (A) The effects of the internal return of return on (purple, left panel) hydrothermal wastewater sludge management cost and (blue, right panel) MDSP. (B) The CI of (red, left panel) hydrothermal wastewater sludge management and (blue, right panel) biofuel production. The left side of each figure is from the waste management perspective, whereas the right side of each figure is from the renewable diesel production perspective. Dotted, dashed, and the middle lines represent 5th/95th, 25th/75th, and 50th percentiles from 1,000 Monte Carlo simulations. Shaded areas in each figure represent (A, left panel) current wastewater sludge management cost (only covers part of the current value [110 to 882 \$·tonne−1] for figure readability), (A, right panel) commercial diesel price range, (B, left panel) current wastewater sludge management CI (only covers part of the current value [−245 to 2200 kg CO₂ eq·tonne⁻¹] for figure readability), and (B, right panel) petroleum diesel production CI.

Table S12. Element (in kg·h−1) and energy (in GJ·h−1) distribution along HTL-based treatment trains for different feedstocks.

a % of C, N, P, or E from the feedstock.

 b % of E from the feedstock and hydrotreating H_2 .

 \degree % of E from the feedstock, hydrotreating H₂, and hydrocracking H₂.

Table S13. Spearman's rank order correlation coefficients for hydrothermal wastewater sludge management (only parameters with p < 0.05 and |ρ| > 0.1 are listed). Indicators include sludge management cost, minimum diesel selling price (MDSP), the carbon intensity of sludge management from the waste management perspective (CIsludge), and the carbon intensity of diesel production from the renewable diesel production perspective (Cldiesel).

a Total organic carbon to total carbon ratio in the HTL aqueous phase.

Feedstock	CFs	ACD	ECO	EUT	OZD	PHO	CAR	NCA	RES		
	unit	$[H^*]$ -eq	kg 2,4-D-eq	kg N-eq	kg CFC-11-eq	kg NO _x -eq	kg benzene-eq kg toluene-eq		kg PM _{2.5} -eq		
	normalized by per tonne waste managed										
Wastewater	5 th	77.8	1630	$-5.46E - 01$	$-1.11E-04$	$3.62E - 01$	1.61	5790	$3.52E - 01$		
	median	157	2610	$-4.13E - 01$	$-6.45E-05$	$9.38E - 01$	3.38	10600	7.14E-01		
	95 th	274	4470	$-2.81E - 01$	$-1.75E-05$	1.80E+00	5.06	16600	$1.24E + 00$		
sludge	normalized by per MMBTU diesel produced ^a										
	5 th	14.9	196	$-3.78E - 02$	$4.77E - 06$	8.59E-02	$1.67E - 01$	804	$6.39E - 02$		
	median	26.2	330	$-2.41E-02$	$8.52E - 06$	$1.67E - 01$	$4.42E - 01$	1390	$1.19E - 01$		
	95 th	42.8	574	$-8.91E - 03$	$1.39E - 05$	$2.85E - 01$	$6.96E - 01$	2300	$1.93E - 01$		
					normalized by per tonne waste managed						
	5 th	23.2	1580	$-4.56E - 01$	$-2.93E - 04$	$-1.45E - 01$	3.81	6490	$-1.74E - 01$		
	median	104	2390	$-3.01E - 01$	$-1.97E - 04$	$5.13E - 01$	4.35	8340	3.28E-01		
FOG	95 th	234	3790	$-1.34E - 01$	$-9.75E - 05$	1.35E+00	5.00	11600	$8.92E - 01$		
	normalized by per MMBTU diesel produced ^a										
	5 th	7.07	79.3	$6.85E - 03$	$3.88E - 06$	$3.88E - 02$	$1.95E - 01$	372	$1.61E - 02$		
	median	11.8	121	$1.25E - 02$	$7.12E - 06$	7.69E-02	2.28E-01	480	4.50E-02		
	95 th	17.7	199	$2.02E - 02$	$1.13E - 05$	$1.19E - 01$	$2.66E - 01$	645	7.26E-02		
	normalized by per tonne waste managed										
	5 th	140	2080	$-3.67E - 01$	$-1.27E - 04$	7.73E-01	4.44	15500	$6.29E - 01$		
	median	231	3220	$-2.40E - 01$	$-6.86E - 05$	1.44E+00	6.20	23700	$1.07E + 00$		
Food waste	95 th	389	5360	$-1.04E - 01$	$-1.08E - 05$	$2.44E + 00$	8.31	33100	1.63E+00		
					normalized by per MMBTU diesel produced ^a						
	5 th	20.6	214	$-9.73E - 03$	$4.80E - 06$	$1.27E - 01$	$4.53E - 01$	1640	8.96E-02		
	median	32.3	364	$2.18E - 03$	$9.15E - 06$	$2.12E - 01$	$6.92E - 01$	2660	$1.48E - 01$		
	95 th	53.3	630	$1.42E - 02$	$1.47E - 05$	$3.48E - 01$	$9.95E - 01$	4030	$2.31E - 01$		
					normalized by per tonne waste managed						
Green	5 th	241	2570	$-4.69E - 02$	$-5.28E - 05$	1.61	5.98	23100	1.12		
waste	median	324	3870	$5.02E - 02$	$-4.47E-05$	2.18	8.06	33700	1.47		
	95 th	490	6460	$1.63E - 01$	4.80E-05	3.26	10.2	45200	2.04		

Table S14. Life cycle environmental impact results across feedstocks and categories.

a The normalization for diesel produced did not account for environmental impacts offset by avoiding traditional waste management methods.

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