Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary Information for

Energy positive domestic wastewater treatment: The roles of anaerobic and phototrophic technologies

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Section S1. Methodology for Inclusion in Review and Results

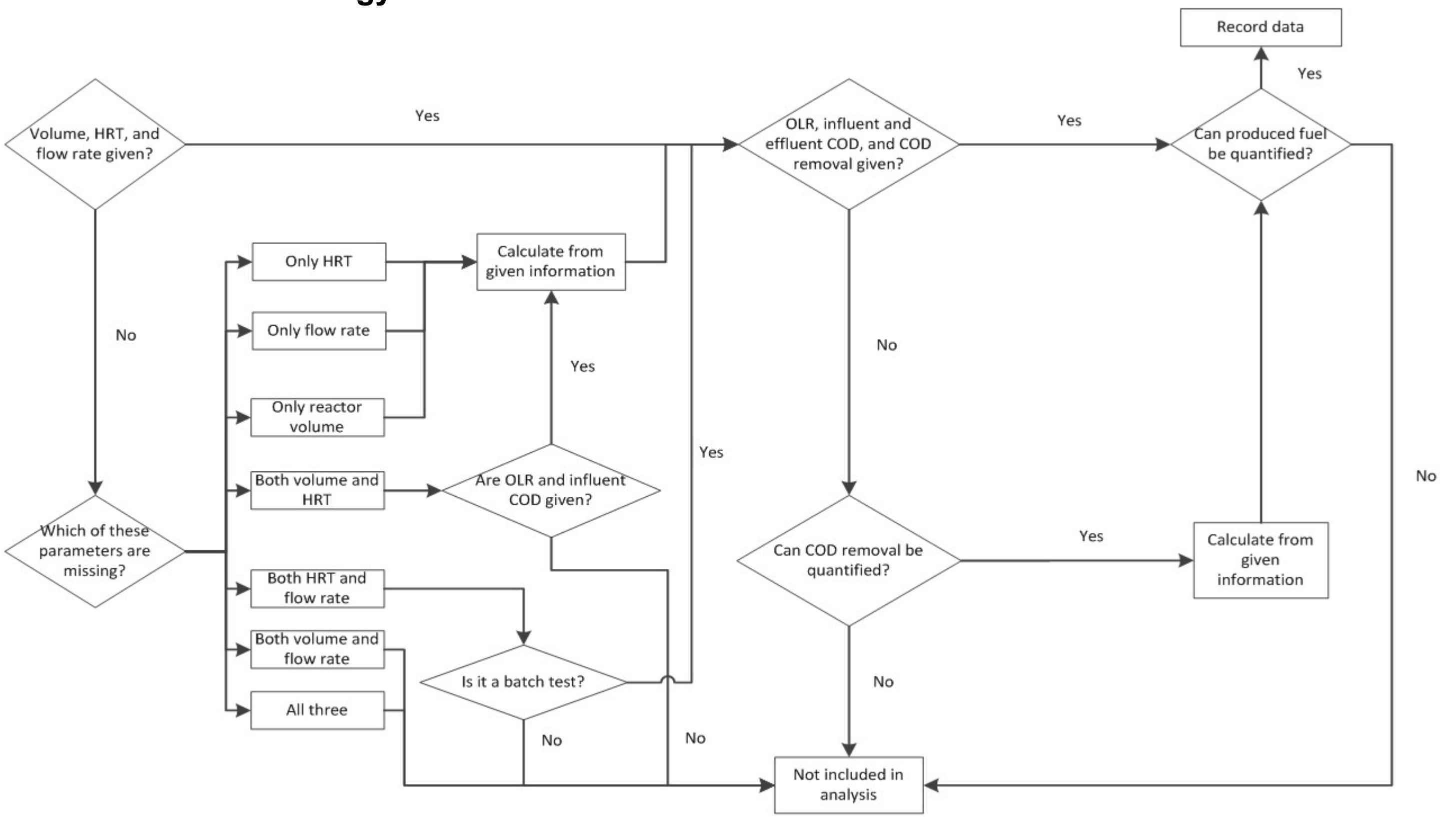


Figure S1. Decision tree for anaerobic data. This methodology was followed to determine if a manuscript examining an anaerobic technology had sufficient data to be included in the review.

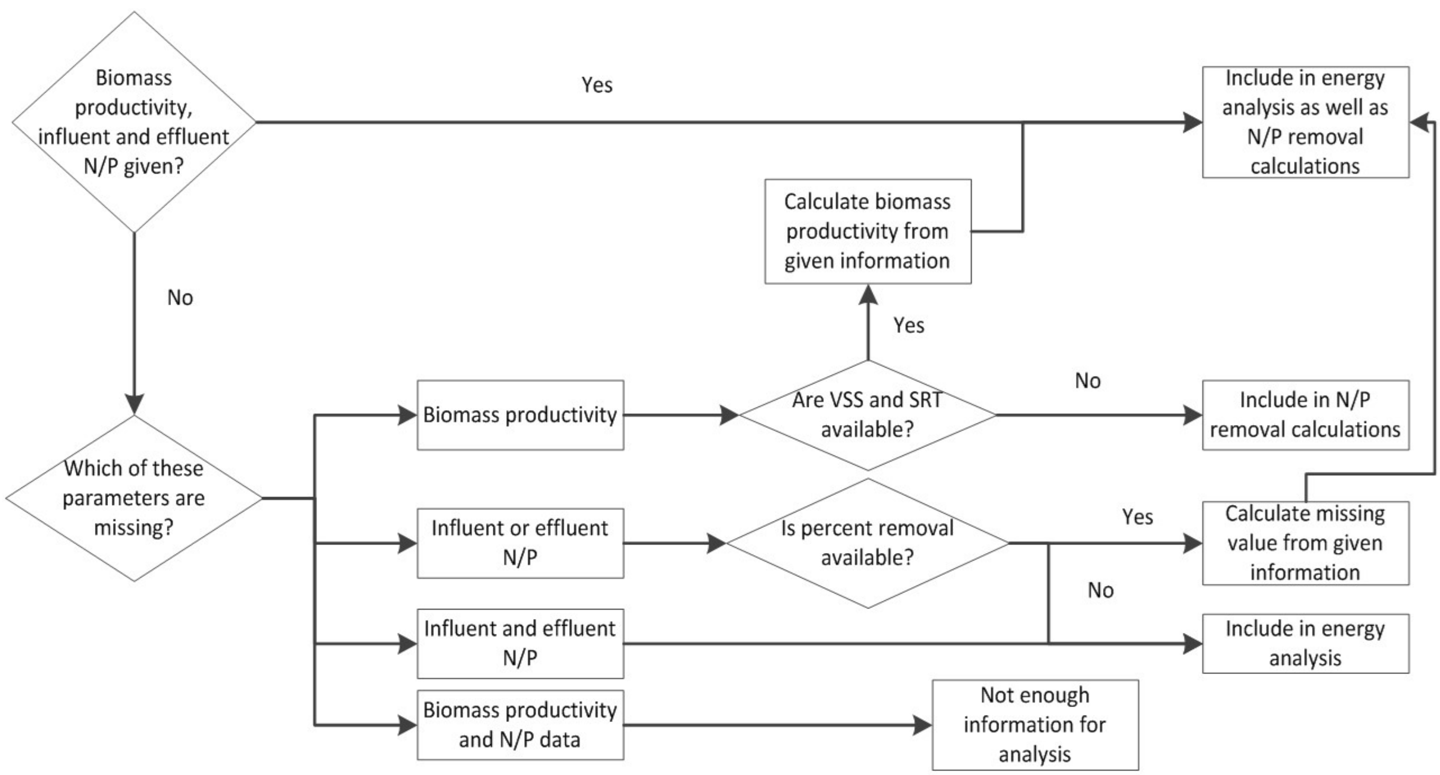


Figure S2. Decision tree for phototrophic data. This methodology was followed to determine if a manuscript examining a phototrophic technology had sufficient data to be included in the review.

Table S1. Technologies examined in this review for both anaerobic and phototrophic systems, and the number of published studies included and the respective citations for each.

Technology	Number of Published Studies	Citations
ASBR	4	1–4
UASB	4	5–8
ABR	3	9–11
AFB	5	12–16
AnMBR	6	17–22
MEC	7	23–29
MFC	4	24,30–32
HRAP	7	33–39
PBR	2	39,40
Stirred Tank	8	41–48
WSP	5	49–53
ATS	2	54,55

Section S2. Energy Production

S2.1 Energy Normalization Equations

$$\left(\frac{\text{X mol CH}_4}{}\right)\left(\frac{803\text{ kJ}}{1\text{ mol CH}_4}\right) \qquad \text{(Equation S1)}$$

$$\left(\frac{\text{X mol H}_2}{}\right)\left(\frac{286\text{ kJ}}{1\text{ mol H}_2}\right) \qquad \text{(Equation S2)}$$

$$\left(\frac{\text{X kWh}}{}\right)\left(\frac{3600\text{ kJ}}{1\text{ kWh}}\right) \qquad \text{(Equation S3)}$$

S2.2 Assumptions for Anaerobic and Phototrophic Energy Normalization/ Conversion to Usable Energy

Table S2. Key assumptions utilized when converting from output fuel (anaerobic) or produced biomass (phototrophic) to energy

Parameter	Value	Citation
Energetic content of methane	803 $kJ \cdot mol^{-1}$	56
Energetic content of hydrogen gas	286 $kJ \cdot mol^{-1}$	57
Gas conversion efficiency (using fuel cell)	42.3%	58
N/P limited determination (Redfield ratio)	<16 is N limited	59
Low COD/VSS ratio	1.47 $g\ COD \cdot g\ VSS^{-1}$ 10/40/50% Lipids/Carbs/Proteins	59–63
High COD/VSS ratio	1.84 $g\ COD \cdot g\ VSS^{-1}$ 30/20/50% Lipids/Carbs/Proteins	59–62
Lipid storage compound	Stearic acid ($C_{18}H_{36}O_2$)	64
Carbohydrate storage compound	Glucose ($C_6H_{12}O_6$)	64
Protein compound	$C_{16}H_{24}O_5N_4$	65
Energy content of COD	3.86 $kWh \cdot kg\ COD^{-1}$	66
Low biocrude yield	25%	67
High biocrude yield	54%	68
Higher heating value for microalgae (HTL)	33.2 $MJ \cdot kg^{-1}$	69
Lipid content of algal cells	10-30%	49
Energy content of biodiesel	37.2 $MJ \cdot kg^{-1}$	49
Low methane production from algae digestion	0.1 $L\ CH_4 \cdot g\ VSS^{-1}$	70
High methane production from algae digestion	0.49 $L\ CH_4 \cdot g\ VSS^{-1}$	71
Combustion energy yield	14.2-21.4 $MJ \cdot kg^{-1}$	72,73
Combustion efficiency	70%	49
COD production$\cdot capita^{-1} \cdot d^{-1}$	180	74
N production$\cdot capita^{-1} \cdot d^{-1}$	13	74
P production$\cdot capita^{-1} \cdot d^{-1}$	2.1	74

S2.3 Energy Normalization Results

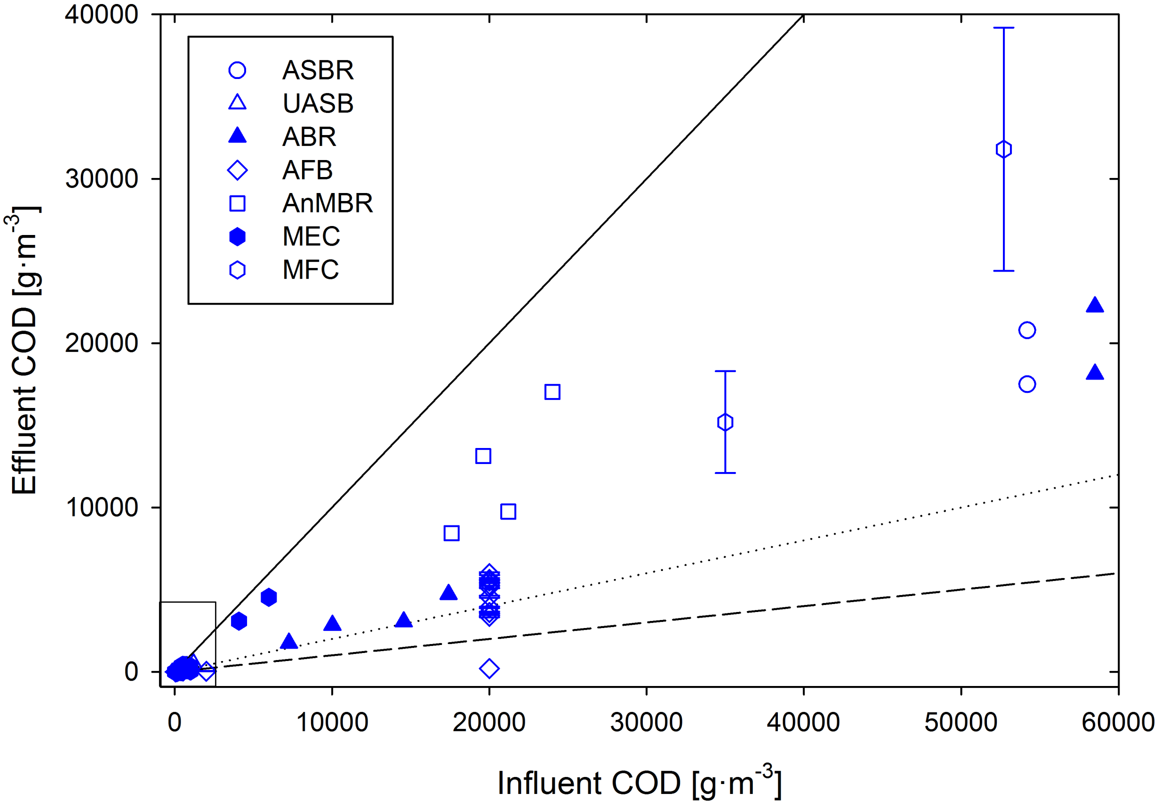


Figure S3. Influent vs. effluent COD [g·m^{-3}] for each paper focusing on anaerobic treatment. Marker shape indicates technology type (e.g. suspended growth, sludge blanket, etc.). The solid line is no COD removal, the dotted line is 80% removal, and the dashed line is 90% removal. The box near the origin is the area examined in Figure 3 signifying influent CODs around 500 mg·L^{-1}.

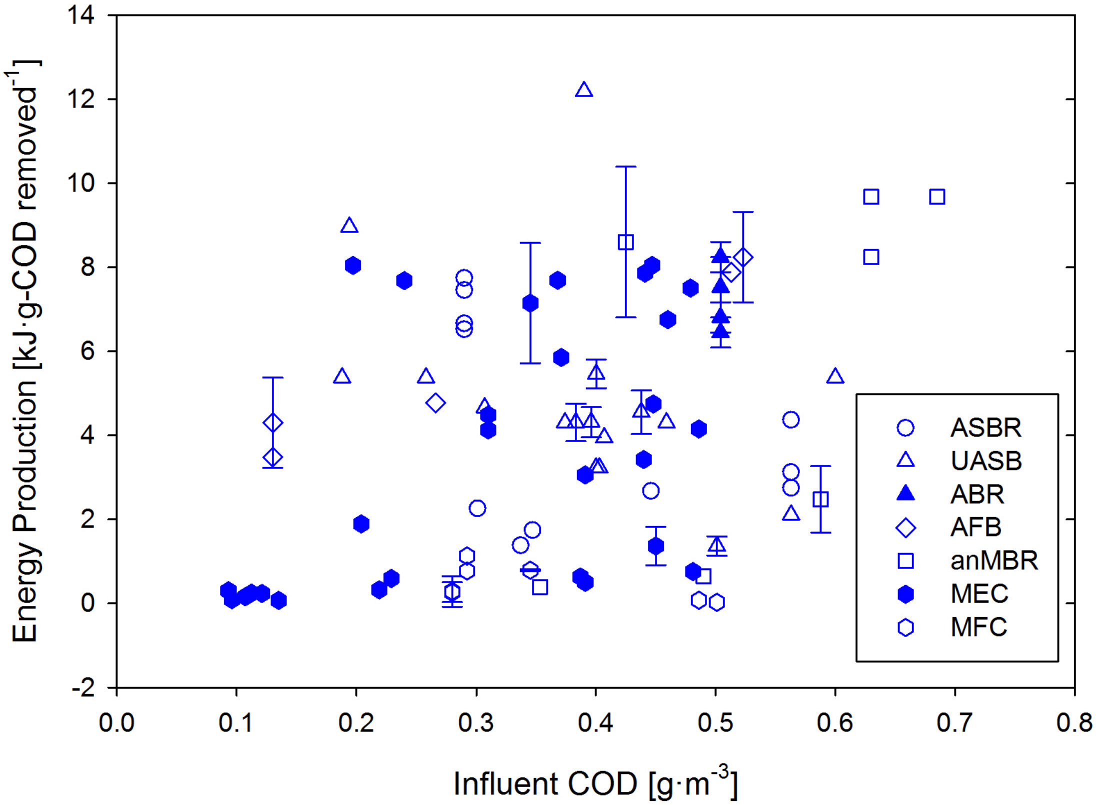


Figure S4. Energy production [$kJ \cdot g\text{-}COD\ removed^{-1}$] vs. influent COD [$g \cdot m^{-3}$] for each paper studying anaerobic technologies with an influent COD below 500 $mg \cdot L^{-1}$ (for synthetic wastewater) or using actual domestic wastewater.

Section S3. Energy Production

S3.1 Theoretical Maximum Energy Production for Anaerobic Technologies

Theoretical maximum energy from anaerobic processes was calculated first by determining the moles of electrons present in the oxidation of 1 kg of oxygen gas to water (see below) [75].

$$\frac{1}{4}O_2 + H^+ + e^- \rightarrow \frac{1}{2}H_2O$$

$$\left(\frac{1\text{ kg COD}}{}\right)\left(\frac{10^3\text{ g}}{1\text{ kg}}\right)\left(\frac{1\text{ mol }O_2}{32\text{ g }O_2}\right)\left(\frac{4\text{ mol }e^-}{1\text{ mol }O_2}\right) = \frac{125\text{ mol }e^-}{1\text{ kg COD}}$$ (Equation S4)

Once this was determined, the 125 moles of electrons were then converted to energy using thermodynamic half reactions [75] as follows:

Methane:

$$\frac{1}{8}CO_2 + H^+ + e^- \rightarrow \frac{1}{8}CH_4 + \frac{1}{4}H_2O$$

$$\left(\frac{125\text{ mol }e^-}{1\text{ kg COD}}\right)\left(\frac{1\text{ mol }CH_4}{8\text{ mol }e^-}\right)\left(\frac{22.4\text{ L }CH_4}{1\text{ mol }CH_4}\right)\left(\frac{35{,}845\text{ kJ}}{1000\text{ L }CH_4}\right) = \frac{12{,}500\text{ kJ}}{1\text{ kg COD}}$$ (Equation S5)

Hydrogen gas:

$$H^+ + e^- \rightarrow \frac{1}{2}H_2$$

$$\left(\frac{125\ \text{mol e}^-}{1\ \text{kg COD}}\right)\left(\frac{1\ \text{mol H}_2}{2\ \text{mol e}^-}\right)\left(\frac{286\ \text{kJ}}{1\ \text{mol H}_2}\right) = \frac{17{,}800\ \text{kJ}}{1\ \text{kg COD}}$$

(Equation S6)

Electricity:

$$dG = -\text{emf}\cdot n \cdot F$$

$$dG = -0.69\ \text{V}\left(\frac{125\ \text{mol e}^-}{1\ \text{kg COD}}\right)\left(\frac{96485.3\ \text{C}}{1\ \text{mol e}^-}\right)\left(\frac{1\ \text{kJ}}{10^3\ \text{J}}\right) = \frac{8300\ \text{kJ}}{1\ \text{kg COD}}$$

(Equation S7)

where dG is the Gibbs free energy, emf is the electromotive force of a microbial fuel cell at open circuit (0.69 V, [76]), n is moles of e^-, and F is Faraday's constant (96485.3 C·mol e^{-1}).

S3.2 Energy Production for Phototrophic Processes

The average energy production per g-N removed by each technology was as follows (average ± standard deviation; largest to smallest): PBR (760 ± 250 kJ·g-N^{-1}), ATS (300 ± 160 kJ·g-N^{-1}), and HRAP (210 ± 96 kJ·g-N^{-1}). The average energy production per g-P removed was as follows: HRAP (2,000 ± 1,300 kJ·g-P^{-1}), Stirred Tank (2,500 ± 1600 kJ·g-P^{-1}), ATS (1,600 ± 780 kJ·g-P^{-1}), and PBR (640 ± 180 kJ·g-P^{-1}).

Section S4. Energy Consumption

S4.1 Mechanical Mixing

$$G = \sqrt{\frac{P}{\mu_w V_r}}$$

(Equation S8)

where G is the mixing intensity, μ_w is the viscosity of wastewater (N·s·m^{-2}), P is power (W), and V_r is volume of the reactor (m^3).

S4.2 Gas Sparging

$$P_w = \frac{wRT_1}{29.7ne}\left[\left(\frac{p_2}{p_1}\right)^{0.283} - 1\right]$$

(Equation S9)

where P_w is the power requirement (kW), w is the weight flow rate of air – volumetric flow rate of air, Q_a, times specific weight – (kg·s^{-1}), R is the engineering gas constant for air (8.314 kJ·$kmol^{-1}$·K^{-1}, T_1 is the absolute inlet pressure (K), p_1 is the absolute inlet pressure (atm), p_2 is the absolute outlet pressure (atm), n is 0.283, and e is the efficiency (0.80)[56].

For phototrophic systems, the flow rate Q_a necessary to obtain well-mixed algal cultures is assumed to be between 0.1 and 0.3 L_{air}· $L_{reactor}^{-1}$·min^{-1}.[77,78]

S4.3 Paddlewheel Operation

We assume 0.037 kW·paddle $wheel^{-1}$ and 11,668 MJ·$hectare^{-1}$·year, with 10 paddles per hectare[79].

S4.4 Harvesting

Harvesting was calculated using reported energy values from Sturm and Lamer 2011[49] that included comparisons to Lardon et al.[80], Batan et al.,[81] and Stephenson et al.[82]. In all cases, the energy consumption was greater for Sturm and Lamer, and these have been chosen as conservative estimates for coagulation/flocculation, dewatering (belt filter press), and centrifugation. A low estimate was chosen as a combination of coagulation/flocculation and belt filter press for dewatering, while the high range was centrifugation (assuming only gravity settling beforehand). Values from Sturm and Lamer are as follows:

Coagulation/flocculation (1 HP/2500 gpm skimmer; 70% efficiency (FRC Systems International, Cumming, GA)): 84 $kWh{\cdot}d^{-1}$

Dewatering (Based on a 250-cm belt width (Komline-Sanderson Model GRS-1)): 340 $kWh{\cdot}d^{-1}$

Centrifugation: 2,080 $kWh{\cdot}d^{-1}$

Normalizing these values for the theoretical plant in Sturm and Lamer (12 MGD treated) and converting to Joules, these values become:

Coagulation/flocculation: 6.66 $kJ{\cdot}m^{-3}$
Dewatering: 26.9 $kJ{\cdot}m^{-3}$
Centrifugation: 165 $kJ{\cdot}m^{-3}$

S4.5 Pumping (Draw-down, Permeate, and Recirculation)

The total dynamic head (TDH) is comprised of the static head (H_{ts}), the friction head (H_{sf}, H_{df}), and minor losses (H_m). For AnMBRs, permeate pumping must also be considered by including transmembrane pressure (TMP). TDH can then be calculated by the equation below:

$$TDH = H_{ts} + H_{sf} + H_{df} + H_m (+TMP) \quad \text{(Equation S10)}$$

However, because minor losses are insignificant compared to the static and friction heads, H_m can be negated. Terms in the TDH equation are further elaborated below:

Total Static Head, H_{ts} (ft): The total static head of pumping can be calculated by the equation below.

$$H_{ts} = H_{ds} - H_{ss} \quad \text{(Equation S11)}$$

Suction Static Head, H_{ss} (ft): Suction static head of pumping is the elevation difference between the water level in the reactor and the centerline of the permeate pump.

Discharge Static Head, H_{ds} (ft): Discharge static head of pumping is the elevation difference between the centerline of the pump and the centerline of the effluent (where water is discharged). The effluent is assumed to be the highest point, thus setting the hydraulic reference.

Suction Friction Head, H_{sf} (ft): Suction friction head can be estimated using the Hazen- Williams equation. Suction friction head refers to the friction loss caused in the pipes on the suction side.

$$H_{sf} = 3.02 L V^{1.85} C^{-1.85} D^{-1.17} \quad \text{(Equation S12)}$$

where L is the length of the pipe (ft), V is the velocity of the liquid in the pipe ($ft{\cdot}s^{-1}$), D is the inner diameter of the pipe (ft) and C is the Hazen-Williams coefficient (110).

Discharge Friction Head, H_{df} (ft): Discharge friction head refers to the friction loss caused in the pipes on the discharge side. The Hazen- Williams equation is also used to calculate this value.

Transmembrane Pressure, *TMP* (ft): This value is based on is based on the 25th and 75th percentiles of TMP reported in the literature. [19–21,83–88].

Brake Horsepower, *BHP***:** BHP is the amount of horsepower required to drive the pump and can be calculated by the equation below:

$$BHP = \frac{Q \cdot TDH}{3960 \cdot \text{Pump Efficiency}}$$
(Equation S13)

where *Q* is the flow rate (gpm), *TDH* is the total dynamic head (ft), and the pump efficiency is assumed to be 80%.

Energy consumption, *E* (kW): The amount of energy input into the motor of the pump can be calculated as:

$$E = \frac{0.746 \cdot BHP}{\text{Motor Efficiency}}$$
(Equation S14)

where *BHP* is the break horsepower (hp) and motor efficiency is assumed to be 70%.

S4.6 Heating

We can compute the heat requirement for the influent wastewater stream as follows [56]:

$$q = \frac{cm\Delta T}{Q}$$
(Equation S15)

where *q* is heat transfer (kJ·m^{-3}), *c* is the specific heat of the wastewater stream (J·kg^{-1} ·˚C^{-1}), *m* is mass flow rate of wastewater (kg·d^{-1}), *Q* is the flow rate (m^3·d^{-1}) and ΔT is the temperature change (˚C).

S4.7 Assumptions for Energy Consumption Calculations

Table S3. Assumptions associated with each of the energy-consuming processes listed above along with values and citations thereof.

Assumption	Value	Citation
General		
Influent pumping	0 m^3·d^{-1}	-
HRT	1 day	-
Influent flow rate	1,000 m^3·d^{-1}	-
Influent COD	500 mg·L^{-1}	66
Influent N	36 mg·L^{-1}	66
Influent P	5.8 mg·L^{-1}	66
Specific heat of wastewater	4.2 kJ·kg^{-1}·˚C^{-1}	56
Density of wastewater (20˚C)	998.2063 kg·m^{-3}	89
Viscosity of water	8.9x10^{-4} N·s·m^{-2}	89
Specific weight of water (20˚C)	1.20 kg·m^{-3}	56
Pipe internal diameter	1 ft	-
Mixing		
Mixing intensity, ASBR	250-350 s^{-1}	-
Mixing intensity, Stirred Tank	100-200 s^{-1}	-

Gas Sparging		
Weight flow of air	13-19 $kg\cdot s^{-1}$	[84,85]
Temperature	20˚C	-
Outlet pressure	1.4 atm	-
Efficiency	80%	[56]
Aeration		
Weight flow of air	2-4 $kg\cdot s^{-1}$	-
Temperature	20˚C	-
Outlet pressure	1.4 atm	-
Efficiency	80%	[56]
Paddlewheel Operation		
Number of paddlewheels	1-3	-
Area of reactor	3030.3 m^2	-
Depth	0.33 m	-
Recirculation Pumping		
Total static head	2 ft	-
Suction friction head length	30 ft	-
Discharge friction head length	120 ft	-
Flow rate for BHP calculation	5x Influent flow	-
Velocity in pipes	3-6 $ft\cdot s^{1}$	-
Recirculation Rate	4.4-386.6	[14]
Effluent Pumping		
Total static head	5 ft	-
Suction friction head length	30 ft	-
Discharge friction head length	30 ft	-
Flow rate for BHP calculation	Influent flow	-
Velocity in pipes	3-6 $ft\cdot s^{-1}$	-
Permeate Pumping		
Total static head	2 ft	-
Suction friction head length	30 ft	-
Discharge friction head length	30 ft	-
Flow rate for BHP calculation	Influent flow	-
Velocity in pipes	3-8 $ft\cdot s^{-1}$	-
Heating[a]		
Influent temperature	18-23˚C	-
Desired heating temperature	35˚C	-
Heat transfer efficiency	100%	-
Applied Voltage		
Applied Voltage	0.5-1.2 V	[26]

[a] For the anaerobic processes, heating occurs before the influent flow

S4.8 Conversion Efficiencies for Biomass to Fuel Processes

Table S4. Energy yield capabilities of biomass conversion processes indicating resulting fuel.

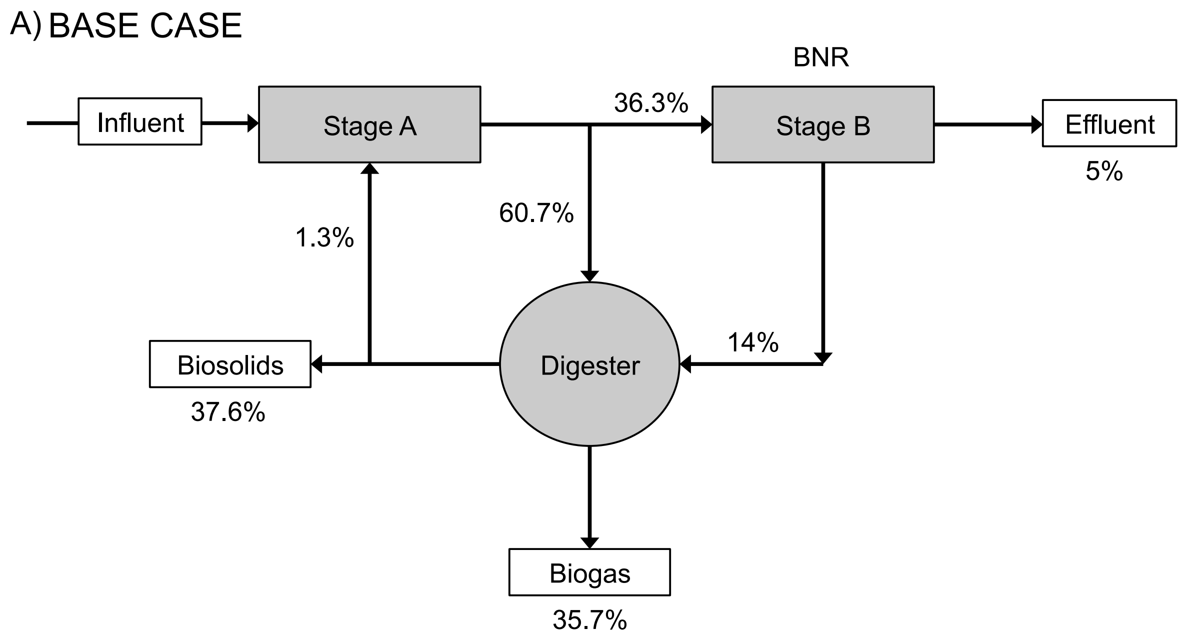
Conversion	Fuel Type	Energy Content [MJ·kg fuel^{-1}]	Conversion Efficiency [% of Biomass Converted to Fuel]	Low Energy Yield [MJ]	High Energy Yield [MJ]	Citation
Caloric Content	Biomass	20.4-25.6[a]	100%	20.4	25.6	Calculated
Hydrothermal Liquefaction	Crude Oil	33.2	25-54%	8.3	17.9	69
Anaerobic Digestion	Methane	35.8	40-60%[b]	3.59	17.6	56,71,90
Transesterification	Biodiesel	37.2	10-30%[c]	3.72	11.16	49,69
Combustion	Biomass	14.2-21.4	70%	9.9	15	72,73

[a] Calculated from COD content assuming low and high composition (10 and 30% lipid) as listed in the manuscript and a theoretical 13.9 kJ·g COD^{-1} oxidized to CO_2 and H_2O[91]
[b] Estimated conversion efficiency of anaerobic digestion on algal VSS only[71]. For calculations, conversions of 0.1 and 0.49 m^3 CH_4·kg VSS^{-1} used[71]
[c] Lipid content, assumed 100% conversion of lipids to biodiesel[49,63]

Table S5. Energy consumption of technologies shown in Table 2, converted to kJ/g nutrient removed for ease of comparison to energy yields in Table 4

Technology	E [kJ]·day^{-1} (low)	E [kJ]·day^{-1} (high)	E [kJ]·g N removed^{-1} (low)	E [kJ]·g N removed^{-1} (high)	E [kJ]·g P removed^{-1} (low)	E [kJ]·g P removed^{-1} (high)
HRAP	37,200	179,600	2	7	12	59
PBR	638,9000	13,228,000	226	468	1,181	2,446
Stirred Tank	832,000	3,301,000	37	147	183	728
WSP	3,400	170,000	N/A	N/A	N/A	N/A
ATS	0	0	0	0	0	0

Section S5. Treatment system based energy simulation for the Strass, Austria wastewater treatment plant



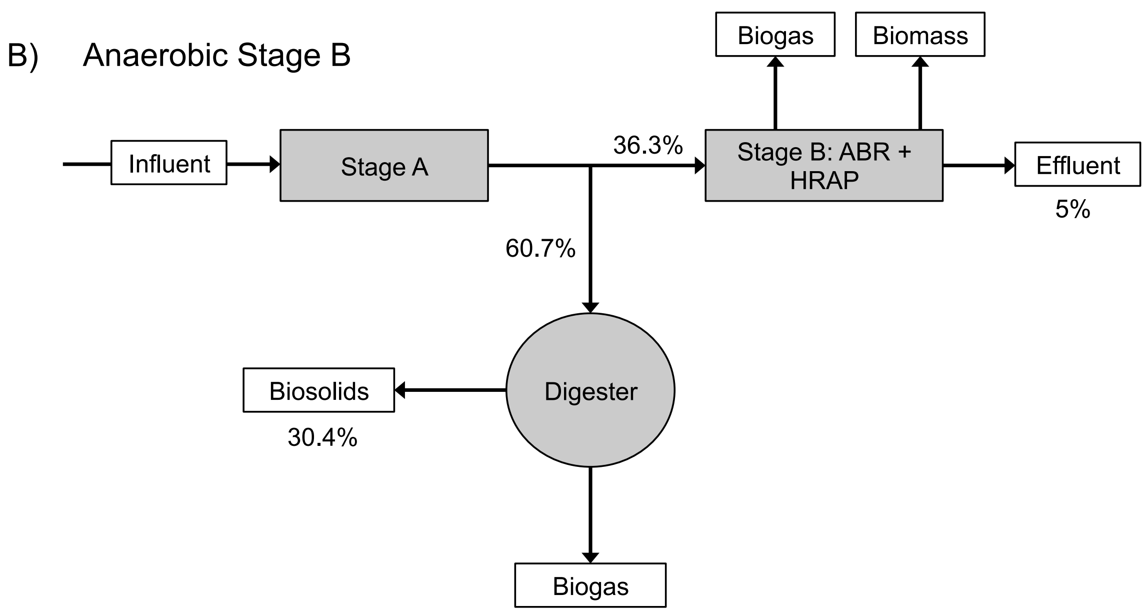


Figure S5. Process flow diagrams of the Strass wastewater treatment plant. A) Base Case: Currently the plant employs aerobic biological nutrient removal (BNR) to treat the liquid stream. B) Anaerobic Stage B: If the BNR stage was converted to a two stage process involving COD removal in a anaerobic baffled reactor (ABR) and nutrient removal in a high rate algal pond (HRAP), COD and nitrogen removal would result in the production of biogas and biomass. The percentages refer to the COD mass balance within the plant.

Table S6. Simulated energy consumption, recovery and production associated with COD and N removal at the Strass wastewater plant. Refer to Figure S5 for more detail.

Condition	Stage B Energy (kJ·Cap^{-1})		Digester Biogas (kJ·Cap^{-1})	Total (kJ·Cap^{-1})
	COD	NH_3-N		
BNR	-140		740	600
ABR + HRAP	420	2,200	600	3,200
ABR + PBR	420	7,900	600	8,900

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