Supplementary Information for

Turning Sewage Sludge and Medical Waste into Energy: Sustainable Process Synthesis via Surrogate-

based Superstructure Optimization

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Number of Pages: 17 6 Tables: Tables S1-S7 10 Figures: Figures S1-S10 26 Equations: Equations S1-S26

Proximate analysis (wt.%)			Ultimate analysis (wt.%)				HHV		
Moisture	Ash	Volatiles	Fixed carbon	С	Н	0	Ν	S	(MJ/kg)
4.53	15.01	68.57	16.42	45.25	6.28	28.26*	5.20	0	24.42
5	0.2	92.9	1.9	84.17	14.93	0.7	0	0	46.9
	I Moisture 4.53 5	Proximat Moisture Ash 4.53 15.01 5 0.2	Proximate analysis (Moisture Ash Volatiles 4.53 15.01 68.57 5 0.2 92.9	Proximate analysis (wt.%)MoistureAshVolatilesFixed carbon4.5315.0168.5716.4250.292.91.9	Proximate analysis (wt.%) Ul Moisture Ash Volatiles Fixed carbon C 4.53 15.01 68.57 16.42 45.25 5 0.2 92.9 1.9 84.17	Proximate analysis (wt.%) Ultimate a Moisture Ash Volatiles Fixed carbon C H 4.53 15.01 68.57 16.42 45.25 6.28 5 0.2 92.9 1.9 84.17 14.93	Proximate analysis (wt.%) Ultimate analysis (wt.%) Moisture Ash Volatiles Fixed carbon C H O 4.53 15.01 68.57 16.42 45.25 6.28 28.26* 5 0.2 92.9 1.9 84.17 14.93 0.7	Proximate analysis (wt.%) Ultimate analysis (wt.%) Moisture Ash Volatiles Fixed carbon C H O N 4.53 15.01 68.57 16.42 45.25 6.28 28.26* 5.20 5 0.2 92.9 1.9 84.17 14.93 0.7 0	Proximate analysis (wt.%) Ultimate analysis (wt.%) Moisture Ash Volatiles Fixed carbon C H O N S 4.53 15.01 68.57 16.42 45.25 6.28 28.26* 5.20 0 5 0.2 92.9 1.9 84.17 14.93 0.7 0 0

Table S1. Characteristics of sewage sludge and medical waste (dry basis) ^{1,2}.

* Calculated by difference.

S1. Unit model development

S1.1 Plasma gasification

The plasma gasification process can be divided into three primary stages: drying, decomposition, and gasification. As illustrated in Figure S1, each stage is represented in Aspen Plus by specific modules designed to precisely simulate the reactions and processes occurring in that phase. Specifically, "*RStoic*" module, "*RYield*" module and "*RGibbs*" module are employed to model the drying, decomposition, and gasification phase, respectively ³. In the drying process, well-established stoichiometric reactions of waste de-water is used ⁴. Within the decomposition stage, the unconventional waste materials are decomposed into elemental components quantified by the ultimate analysis results of the waste (as illustrated in Table S1), which allows for precise simulation via a yield reactor. In the gasification phase, steam and air are ionized to plasma state using a plasma torch (modeled by a heat exchanger) to serve as gasifying agents. The essential chemical reactions that drive this phase are detailed in Equations S1-S5. By employing the "*RGibbs*" module is employed here to achieve chemical and phase equilibrium by minimizing Gibbs free energy within the system ^{5,6}. The intense heat generated in the plasma gasification stage ensures complete conversion of organic volatiles. Any resulting solid residue is separated by a cyclone, while the high-temperature crude syngas is harnessed to preheat the feedstock.

$$C + H_2 0 \rightleftharpoons CO + H_2 \tag{S1}$$

$$C + CO_2 \rightleftharpoons 2CO \tag{S2}$$

$$CO + H_2 O \rightleftharpoons CO_2 + H_2 \tag{S3}$$

$$CH_4 + H_2 0 \rightleftharpoons CO + 3H_2 \tag{S4}$$

$$C + O_2 \rightleftharpoons CO_2 \tag{S5}$$



Figure S1. Flowsheet of plasma gasification.

Plasma gasification is a critical unit operation within the superstructure, playing a significant role in the overall process. Due to the lack of detailed kinetic-based models for gasification, equilibrium models relying on Gibbs minimization have been commonly used ^{5,6}. Given the simplified nature of these models, validation is essential. In this work, the developed model is validated using data from previous plasma gasification studies ⁷. The simulation outcomes generated by this model, with various feedstocks, are then compared with existing literature on plasma gasification. Figures S2 and S3 display the primary syngas components, i.e., H₂ and CO. To quantitatively assess the model's accuracy, the root mean square error (RMSE) is employed. The H₂ and CO fractions predicted by our model closely align with those reported in the literature, with low RMSE values of 0.0115 and 0.0101, respectively. These findings indicate that the developed model is effective in accurately predicting syngas composition of the plasma gasification process.



Figure S2. Comparison results for H₂ derived from plasma gasification of different feedstocks.



Feedstocks



The produced syngas by plasma gasification is subsequently cooled and routed to the water gas shift (WGS) reactor, which is simulated using a adiabatic "*RPlug*" module integrated in Aspen Plus. Due to the simplicity and extensive study of the WGS reaction, a well-established kinetic-based plug flow reactor model with a power-lar kinetic expression is employed for simulation. For the high-temperature WGS reactor, the reaction rate ($r_{HT} - WGS$) is determined using Equation S6 ^{8–10}. The reaction rate for the low-temperature WGS reactor ($r_{LT} - WGS$) is similarly modeled, as shown in Equation S7 ¹¹.

$$r_{HT-WGS} = k_{HT} \times exp^{[iii]}(-E_{HT}/RT) \times P_{CO} \times P_{CO_2}^{-0.36} \times P_{H_2}^{-0.09} \times (1 - (P_{CO_2} \times P_{H_2})/(P_{CO} \times P_{H_2} \times K_{HT}))$$
(S6)

$$r_{LT - WGS} = k_{LT} \times exp^{[m]}(-E_{LT}/RT) \times (P_{CO} \times P_{H_2O} - (P_{CO_2} \times P_{H_2}/K_{LT}))$$
(S7)

where k_{HT} and E_{HT} represent the kinetic factor and apparent activation energy of the high-temperature WGS reaction with values of $10^{2.845}$ mol·s⁻¹·g⁻¹·Pa^{-0.55} and 111 kJ·mol⁻¹, respectively ^{8,9}. K_{HT} donates the equilibrium constant of the high-temperature WGS reaction while R is the molar gas constant. P_{CO_2} , P_{H_2} , P_{CO} and P_{H_2} indicate the partial pressure of CO₂, H₂, CO and H₂. k_{LT} and E_{LT} the kinetic factor and apparent activation energy of the low-temperature WGS reaction which are equal to 1.612×10^{-5} kmol·s⁻¹·m⁻³·Pa⁻² and 47400 kJ·kmol⁻¹, respectively ^{8,11}. The equilibrium constant of the low-temperature WGS reaction is donated by K_{LT} .

S1.3 Methanol synthesis

Figure S4 illustrates the methanol synthesis unit's process flow. The upgraded syngas is compressed and heated before entering the reactor. A purge stream, mixed with tail gases, is utilized to manage the accumulation of inert gases in the reactor and regulate the recycle stream. The reactions considered in the model are detailed in Equations S8-S9¹². To enhance energy efficiency, the crude methanol produced is used to preheat the incoming feedstock for this unit. And then further separation is required to achieve a high-purity methanol product which is accomplished through a distillation process. The first distillation column removes

most of the light gases, while the second column separates water from the methanol-water mixture. Both columns are simulated using the rigorous "*Radfrac*" module, with tail gases collected in a partial condenser. For the first methanol synthesis configuration (FP2), a kinetic model with established parameters is employed, using the widely accepted kinetic description provided in Equations S10-S11¹³. In contrast, the second methanol synthesis configuration (FP3) uses a simplified conversion rate-based reactor model ¹⁴.

$$CO_2 + 3H_2 \rightleftharpoons CH_3 OH + H_2 O \tag{S8}$$

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \tag{S9}$$

$$r_{1} = (k_{1}P_{CO_{2}}P_{H_{2}} - \frac{k_{2}P_{H_{2}}O^{P}_{CH_{3}}OH}{P_{H_{2}}^{3}P_{CO_{2}}})/(1 + \frac{k_{3}P_{H_{2}}O}{P_{H_{2}}} + k_{4}P_{H_{2}}^{0.5} + k_{5}P_{H_{2}O})^{3}$$
(S10)

$$r_{2} = (k_{6}P_{CO_{2}} - \frac{k_{7}P_{H_{2}}O^{P}CO}{P_{H_{2}}P_{CO_{2}}}) / (1 + \frac{k_{3}P_{CO_{2}}}{P_{H_{2}}} - k_{4}P_{H_{2}}^{0.5} + k_{5}P_{H_{2}O})$$
(S11)

where r_1 and r_2 are the kinetic reaction rates of methanol synthesis (Equation S8) and reverse water gas shift (Equation S9). P_{CO_2} , P_{H_2O} , P_{CO} , P_{CH_3OH} and P_{H_2} represent the partial pressure of CO₂, H₂O, CO, CH₃OH and H₂. Kinetic parameters k_1 , k_2 , k_3 , k_4 , k_5 , k_6 and k_7 are described by Equation S12.

$$lnk_i = A_i + B_i/T \tag{S12}$$

where A_i and B_i are kinetic constants of methanol synthesis reactions on the Cu/ZnO/Al₂O₃ catalyst, which are summarized in Table S2.

Table S2. Kinetic constants of methanol synthesis reactions ¹⁵.

Kinetic constants	k_1	k ₂	k ₃	k_4	k ₅	k ₆	k_7
A _i	-29.87	17.55	8.147	-6.452	-34.95	4.804	0.1310
$B_{i/J} \cdot \text{mol}^{-1}$	4811.2	-2249.8	0	2068.4	14928.9	-11797.5	-7023.4



Figure S4. Flowsheet of methanol synthesis.

S1.4 One-step dimethyl ether (DME) synthesis

The upgraded syngas is compressed to a high pressure ¹⁶ and then used for DME synthesis, as illustrated in Figure S5. The process involves the single-step synthesis of DME, which has been reported previously ¹⁶. This reaction sequence includes methanol production from CO, methanol production from CO₂, DME formation, and the water gas shift (WGS) reaction, detailed in Equations S13-S16. A plug flow reactor model is applied for the simulation, with the Langmuir-Hinshelwood Hougen-Watson (LHHW) model describing the reaction kinetics. To conform to the LHHW model, the reaction rates of reactions S13-S16 are expressed as shown in Equations S17-S20 ¹⁶. After cooling via a cooler and removing water removal via a flasher, DME is separated by using distillation. The distillation column is modeled in equilibrium mode with 25 stages ¹⁷. The separated DME, collected from the down of distillation column, serves as a crude product and undergoes further distillation to obtain high-purity DME. The distillate from the top of the column, which contains light gases (mainly unreacted syngas, CO₂, and minor DME), is sent to the tail gas treatment unit.

$$CO + 2H_2 \rightleftharpoons CH_3OH$$
 (S13)

$$CO_2 + 3H_2 \rightleftharpoons CH_3 OH + H_2 O \tag{S14}$$

$$2CH_3OH \rightleftharpoons CH_3OCH_3 + H_2O \tag{S15}$$

$$CO + H_2 O \rightleftharpoons CO_2 + H_2 \tag{S16}$$

$$r_{MS} = \frac{(k_1 f_{CO} f_{H_2}^2 - (k_1 f_{CH_3 OH} / K_{f_1}))}{(1 + k_{CO} f_{CO} + k_{CO_2} f_{CO_2} + k_{H_2} f_{H_2})^3}$$
(S17)

$$r_{MS2} = \frac{(k_2 f_{CO_2} f_{H_2}^3 - (k_2 f_{CH_3 OH} / K_{f2}))}{(1 + k_{CO} f_{CO} + k_{CO_2} f_{CO_2} + k_{H_2} f_{H_2})^4}$$
(S18)

$$r_{DS} = (k_3 f_{CH_3OH} - (k_3 f_{DME} f_{H_2O} / K_{f3} f_{CH_3OH}^2)) / (1 + \sqrt{k_{CH_3OH} f_{CH_3OH}})^2$$
(S19)

$$r_{WGS} = \frac{(k_4 f_{H_20} - (k_4 f_{C0_2} f_{H_2} / K_{f4} f_{C0}))}{(1 + k_{c0} f_{c0} + k_{c0_2} f_{c0_2} + \sqrt{k_{H_2} f_{H_2}})}$$
(S20)

where r_{MS} , r_{RWGS} , r_{DS} , r_{WGS} are the kinetic rates for reactions presented in Equations S13-16. f_{CO} , f_{H_2} , f_{CH_3OH} , f_{CO_2} , f_{DME} and f_{H_2O} are the fugacity of CO, H₂, CH₃OH, CO₂, DME and H₂O, respectively. k_1 , k_2 , k_3 , and k_4 are rate constants while k_{CO} , k_{CO_2} , k_{H_2} and k_{CH_3OH} are adsorption coefficients. They are expressed by Equation S21. The values of parameters A_i and B_i are summarized in Table S3. K_{f1} , K_{f2} , K_{f3} , and K_{f4} are equilibrium constants of reactions S13-S16 which are expressed in Equations S22-S24 ¹⁸.

$$k_i = A_i e^{\binom{B_i/RT}{}}$$
(S21)

$$lnK_{f1} = lnK_{f2} = 4213/T - 5.752 \times lnT - 1.707 \times 10^{-3} \times T + 2.682 \times 10^{-6} \times T^{2} + 17.6$$
(S22)

$$lnK_{f3} = 4019/T - 3.707 \times lnT - 2.783 \times 10^{-3} \times T + 3.8 \times 10^{-7} \times T^{2} + 26.64$$
(S23)

$$lnK_{f4} = 2167/T - 0.2258 \times lnT - 1.037 \times 10^{-3} \times T + 2.331 \times 10^{-7} \times T^{2} + 1.2777$$
(S24)

Table S3. Parameters for kinetic rate constants and adsorption coefficients of reactions involved in DME synthesis ¹⁸.

Kinetic constants	<i>k</i> ₁	<i>k</i> ₂	<i>k</i> ₃	<i>k</i> ₄	k _{CO}	k _{CO2}	k _{H2}	k _{CH3} OH
A _i	7380	5059	1062	7.3976	3.917×10 ⁻⁶	1.858×10 ⁻⁶	0.6716	7.928×10 ⁻⁴



Figure S5. Flowsheet of one-step DME synthesis.

S1.5 Two-step dimethyl ether (DME) synthesis

Figure S6 shows the process flow for the two-step DME synthesis. Initially, the reactant gases are conditioned to match the operating conditions of the methanol synthesis reactor. The upgraded syngas is pressurized using a compressor and then preheated to about 210° C¹⁷ before being introduced into the methanol synthesis reactor. Given the exothermic nature of the methanol synthesis reaction, the produced heat is utilized to preheat the incoming reactants. In this setup, modeled using an "*Rstoic*" reactor, the methanol conversion rate is assumed to be 0.97 mol/mol CO¹⁹. After cooling, the tail gas is separated, and the methanol-rich aqueous solution from the flasher's bottom is directed to a distillation column for purification. The purified methanol is then vaporized and fed into the reactor for the methanol-to-DME conversion, as described by Equation S14. This reaction is also modeled with an "*Rstoic*" reactor, applying specific conversion rates for the reactants. The resulting crude DME is condensed and purified through distillation, while any unreacted methanol is recycled back into the DME synthesis reactor to enhance the overall conversion efficiency.



Figure S6. Flowsheet of two-step DME synthesis.

S1.6 Fischer-Tropsch (FT) synthesis

Figure S7 illustrates the flowsheet for Fischer-Tropsch (FT) fuel synthesis. The upgraded syngas, including hydrogen (H₂) supply, is compressed and introduced into continuous fixed-bed reactors (modeled using two "*RStoic*" blocks) operating at 220°C and 30 bar. Due to the exothermic nature of methanol synthesis, the heat generated is recovered to preheat the incoming reactants via a heat exchanger. The FT synthesis reaction is modeled by incorporating Equation S25 into the reactor model ²⁰. The product distribution follows an Anderson-Schultz-Flory pattern, as shown in Equation S26 ²¹. After the first FT synthesis reactor (reactor 1), the products are cooled to condense heavier hydrocarbons, with the vapor phase (mainly consisting of unreacted syngas and lighter hydrocarbons) being sent to the second reactor. Following cooling of the products from the second reactor (reactor 2), the condensed synfuel is mixed with the product from the first reactor, while unreacted syngas is recycled to the first reactor to improve conversion. To prevent the buildup of inert compounds in the FT gas loop, part of the unreacted gas is routed to a tail gas treatment unit ²⁰. The condensed mixed fuel is then separated by distillation into fuel gases containing unconverted syngas and light

hydrocarbons (C1–C4), which are treated as tail gas, and liquid fuel products, including naphtha, jet fuel, diesel, and wax.

$$nCO + (2n+1)H_2 \rightleftharpoons C_n H_{2(n+1)} + nH_2O$$
(S25)

$$log(W_{n'}n) = n \times log\alpha + log((1-\alpha)^{2}/\alpha)$$
(S26)



Figure S7. Flowsheet of FT synthesis.

S1.7 Tail gas treatment

The tail gases from the fuel production unit still contain combustible components like CO, H_2 , methanol, and DME. To maximize energy recovery, these gases undergo pressurized combustion with air as oxidant, followed by energy recovery operations, as shown in Figure S8. After combustion, the high-temperature and high-pressure flue gas is passed through a gas turbine to generate electricity, reducing the pressure to atmospheric state ²². An organic Rankine cycle (ORC) is then used to capture the remaining lower-grade heat contained in the flue gas, converting it into power via an organic fluid turbine. The cooled flue gas, now primarily composed of N2, H_2O , and CO_2 , undergoes flashing to separate wastewater. The remaining gases are either sent to a CO_2 capture unit or released directly into the atmosphere. Page 11 of 17



Figure S8. Flowsheet of tail gas treatment.

Table S4. Main	operating	conditions and	d parameters	used in	waste-to-energy	processes.
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Units	Parameters	Values	Units
Plasma gasification	Temperature	1560.6 ²³	°C
	Steam-to-waste ratio	0.99 23	-
RWGS ^a	Temperature	1560.6 ²⁰	°C
	Pressure	24.5 ²⁰	bar
	CO ₂ conversion rate	0.36 20	-
Low-temperature WGS	Temperature	200 24	°C
	Pressure	1.013 24	bar
High-temperature WGS	Isentropic efficiency of turbine	400 24	°C
	Pressure	1.013 24	bar
MEA-based CO ₂ capture	Capture efficiency	90 ²⁵	%
	Duty	4.0 ²⁶	MJ/kg
PSA	Energy consumption	0.657 27	kWh/kg feedstock
	H ₂ recovery efficiency	0.85 ³	-
Methanol synthesis1 ^a	Temperature	220 14	°C
	Pressure	55 14	atm

	CO conversion rate	35 14	
	CO ₂ conversion rate	17 14	
Methanol synthesis2	Temperature	240 12	°C
	Pressure	75 12	atm
DME synthesis1	Temperature	280 ¹⁶	°C
	Pressure	60 ¹⁶	bar
DME synthesis2 ^a	Temperature	200 19	°C
	Pressure	50 ¹⁹	atm
	CO ₂ availability	without feeding CO ₂ 19	-
	CO conversion rate	97 ¹⁹	%
	Methanol conversion rate	92 ¹⁹	%
DME synthesis3 ^a	Temperature	200 19	°C
	Pressure	50 ¹⁹	atm
	CO ₂ availability	with feeding CO_2 ¹⁹	-
	CO conversion rate	95 ¹⁹	%
	Methanol conversion rate	91.52 ¹⁹	%
	CO ₂ conversion rate	15 ¹⁹	%
FT synthesis	Temperature	220 ²⁰	°C
	Pressure	30 ²⁰	bar

a: Non-kinetic based models.

Table S5. The price and equivalent emission factor of the materials and utilities.

Items	Prices	Units	Emission factors	Units
processed water	0.001 28	\$/kg	0.0005 29	kg/kg
electricity	0.06 28	\$/kWh	0.6235 28	kg/kWh

fired heat	0.029 28	\$/kWh	0.3406 28	kg/kWh
cooling water	0.00127 30	\$/kWh	0.2984	kg/kWh
low-pressure steam	0.014 28	\$/kWh	0.1875 ²⁸	kg/kWh
high-pressure steam	0.019 28	\$/kWh	0.1875 28	kg/kWh
black H ₂	2.7 28 30	\$/kg	3.5 28	kg/kg
MEA	2.09 ³⁰	\$/kg	0.0656 31	kg/kg
O ₂	40 ²⁹	\$/t	0.038 29	kg/kg
Waste water treatment	4.1 ³²	\$/t	0	kg/kg
LT-WGS catalyst	22000 ³³	\$/t	0.59 31	kg/kg
HT-WGS catalyst	22000 ³³	\$/t	0.59 31	kg/kg
RWGS catalyst	22000 ³³	\$/t	0.59 31	kg/kg
MeOH catalyst	102.77 17	\$/kg	0.59 31	kg/kg
DME catalyst	23.75 17	\$/kg	0.59 ³¹	kg/kg
FT fuel catalyst	69.9 ³⁴	\$/kg	0.59 31	kg/kg

Table S6. Configuration in base case.

Parameters	Values	Units
Waste flowrate	2000	kg/h
MW ratio in feedstock	0.5	-
H ₂ price	5.4 ³⁰	\$/kg
Methanol Price	500 ³⁵	\$/t
DME price	652 ³⁶	\$/t
Naphtha	924 ³	\$/t
Jet fuel	3.24 ³	\$/gal
Diesel	4.13 ³	\$/gal
Wax	2139 ³	\$/t
Carbon tax	0	\$/t CO ₂ -eq



Figure S9. Test results of HDMR models for HC predictions of methanol synthesis processes a) MeOH1 (FP2) and b) MeOH₂ (FP3).



Figure S10. Test results of HDMR models for HC predictions of dimethyl ether synthesis processes a) DME1 (FP4), b) DME2 (FP5) and c) DME3 (FP6).

Items	Input energy/MW	Available energy/MW	Loss energy	Efficiency
Plasma gasification	28.11	20.74	7.37	0.74
Syngas upgrading	20.74	18.18	2.56	0.88
Syngas cleaning	24.56	17.62	6.95	0.72
Fuel production	21.10	19.45	1.64	0.92
Tail gas treatment	4.85	2.40	2.45	0.50
Whole system	40.38	16.02	24.36	0.40

Table S7. Energy balance of the wste-to-H2 process.

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