Supplementary Material

Techno-economic assessment of biological biogas upgrading based on Danish biogas plants

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I. Equiment cost

Equipment cost was calculated by the following equation [1]

$$C_e = a + bS^n$$

where C_e is the equipment cost, S is the equipment size, n is the economy of scale sizing exponent, and a and b are shown in Table S1.

Table S1. Correlation coefficient (a and b) and boundaries values (S_{lower} and S_{upper}) for each equipment type.

Equipment size	Units in the plant	Unit for size, S	S_{lower}	S_{upper}	a	b	n
Floating rooftank	Digester, storage tanks	Capacity, m^3	100	10,000	53,000	2400	0.6
Pressure vessel, 304 stainless steel	Upgrading and desulphurization reactors, hydrogen storage	Shell mass, kg	90	124,200	-10,000	600	0.6
Double pipe heat exchanger	Heat exchangers	Area, m^2	1	80	500	1100	1
Centrifugal single-stage pumps	Pumps	Flow, l/s	0.2	500	3300	48	1.2

For the remaining equipment *i.e.* the packing material and the compressor, the following calculations were carried out. A price of 30 €/m^3 was retrieved from literature [2] and was multiplied by the volume of PUF in the different reactors.
For the compressor, the cost was assessed based on the power using data from Brown et al. [3] and the following equation:

$$C_e = C_{base}\left(\frac{S}{S_{base}}\right)^n$$

Where C_e is the compressor cost, C_{base} is the cost for a compressor with a base size S_{base}, in this case, 1 kW, and n the economy of scale exponent.

Table S2. Equipment cost breakdown

Anaerobic digestion (AD) equipment	€ × 10^3	kr × 10^3
Storage tank for manure	271	2020
Storage tank for industrial waste	168	1254
Pump and mixer	4	29
HEX	8	57
Digester	534	3976
Digestate storage tank	135	1003
Total cost for AD	1119	8338
Desulphurization equipment	€ × 10^3	kr × 10^3
Reactor	244	1818
Packing material	21	159
Total cost for desulphurization	265	1977
	1385	10315
Upgrading equipment	€ × 10^3	kr × 10^3
H_2 storage	539	4018
HEX	2	14
Pump and mixer	70	521
Nutrient storage	45	339
Upgrading reactor	211	1570
Packing material	18	132
Compressor	55	408
Total cost for upgrading	939	7002
Total equipment cost	2324	17317

II. Operational cost

The operational costs were calculated by the following equation

$$OC = \sum_{j=0}^{m} P_j\, Q_j + N_{op}\, S_{op} + \sum_{k=0}^{u} P_k\, Q_k$$

where m is the number of raw materials and P_j is the price of the different raw materials (manure, hydrogen, etc), Q_j is their respective quantities in ton or kg. N_{op} is the number of operators per shift and S_{op} is the salary per hour and per operator, u is the number of utilities and P_k is the price of utilities (electricity, steam, etc) while Q_k is their quantities in kWh or tons/year. The detail of prices is given in the sections below.

Raw materials

The assumptions for the raw material costs are displayed below.

- Manure is assumed to be free of charge whether digestate is sold or not
- Manure transport is assumed to be included in biogas plants costs. An inventory of a few large-scale Danish plants show that the distance to manure suppliers is not higher than 20 km which is a short distance [4]. The price for manure transport is fixed and equal to 2.5 €/ton of manure [5].
- Industrial waste cost is assessed according to the waste management price that companies need to pay but also on suggested prices by other feasibility studies. Industrial waste is set to 30 €/ton [5,6].
- Inoculum and nutrients for AD, desulphurization, and upgrading are assumed to be free of charge. Manure can be used as a nutrient media when prepared adequately [7].
- Oxygen is needed for H_2S removal. Towler et al.[1] indicate an oxygen price of 0.02 USD/lb in 2006 *i.e.* 0.05 €/kg of oxygen in 2019.

Hydrogen cost

Hydrogen is also a raw material however its cost depends on numerous parameters since its production is done via water electrolysis. Hydrogen can be as cheap as 1 to 1.5 €/kg yet NREL (National Renewable Energy Laboratory) and Vo et al. report a price that can be higher than 5 USD/kg (4.5 €/kg) [8,9]. The International Energy Agency in 2017 published a report where the hydrogen cost evolution is given for different electricity prices and full load hours [10].

Fig. S1 illustrates that the price of hydrogen is the lowest when the electricity price is 0 *i.e.* when there is a surplus of electricity. Thus the blue curve corresponds to the price range to consider since the goal of using H_2 is to reduce curtailment caused by electricity overproduction. One assumes that the full load hours is maximum and thus a price of 1.0 €/kg of H_2 is used.

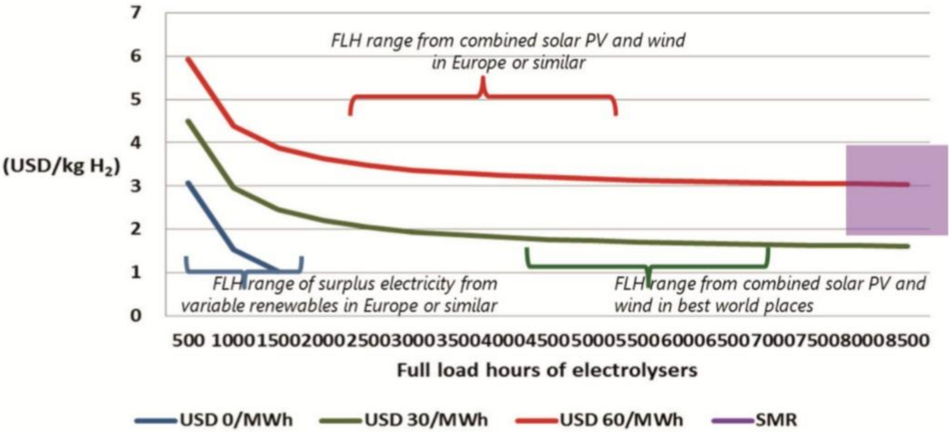

Figure S1. Cost of hydrogen from electrolysis for different electricity costs and load factors [10] Note: Assumptions - Capex of electrolyzers USD 450/kW (Simonsen, 2017), WACC 7%, lifetime 30 years, efficiency 70%; cost of hydrogen from SMR (Steam Reforming) USD 1.0/kgH_2 to USD 3.0/kgH_2 depending on natural gas prices.

Utilities

Biogas heat and electricity needs can be provided by an on-site CHP plant. If it is not the case the electricity can be bought from the grid and other utilities like steam can be provided by an over-the-fence plant. The price of steam, water, and cooling was taken into account in this study case.

- The electricity price for large consumers is lower compared to retail prices. From the first estimation, the plant consumes between 2 and 499 MWh. According to official data from Danish authorities, the electricity price is 0.731 DKK/kWh tax included (0.1 €/kWh) [11].
- Steam and cooling water are retrieved from SuperPro Designer software [12] and are respectively equal to 89.40 DKK/t and 0.37 DKK/t (12 €/t and 0.05 €/m^3)
- Water price is taken from Towler et al. and is equal to 4.53 DKK/m3 (0.61 €/m^3) [1].

Summary of the unit costs for operational expenses

Table S3 summarises all the different unit cost for raw materials, utilities, and operating labor.

Table S3. Unit cost for operational expenses

	Price	Unit
Raw materials		
Manure	0	€/t
Manure transport	2.50	€/t
Industrial waste	30	€/t
Hydrogen	1	€/kg
Inoculum and nutrients	0	€/kg
Oxygen	0.05	€/kg
Utilities		
Electricity	0.098	€/kWh
Steam	12	€/t
Cooling water	0.05	€/m^3
Water	0.61	€/m^3
Operating labor		
Operator	24.2	€/h/operator

Total product cost

On top of the raw materials, operating labor, and utility costs there are other costs incurred to run a plant. These different costs are listed in **Table S4** and details are provided on how these costs are calculated. This cost estimation method is applied for each section of the plant e.g. AD, H_2S removal, and upgrading.

Table S4. Fixed cost calculation factors

	Factor	Basis
Supervision (*S*)	0.25	of operating labor
Direct salary overhead (*DSO*)	0.40	of operating labor and supervision
Maintenance (*M*)	0.03	of TPEC
Property taxes and insurance (*PTI*)	0.015	of FCI
Rent of land and buildings (*RLB*)	0.01	of 83% of FCI
General plant overhead (*GPO*)	0.65	of total labor (incl. supervision, direct overhead, and maintenance)
Allocated environmental burdens (*AEB*)	0.01	of 83% of FCI

The total product cost is calculated by the following equation

$$TPC = M + U + O + S + DSO + MT + PTI + RLB + GPO + AEB$$

and using the factors in Table S4, we have,

$$TPC = M + U + O + 0.25O + 0.4(O+S) + 0.03TPEC + 0.015FCI + 0.01\times 0.83FCI$$
$$+0.65(S + DSO + MT) + 0.1\times 0.83FCI$$

where *M*, *U*, and *O* are respectively the raw materials, the utility, and the operating labor costs.

Tax, depreciation, inflation, and minimum rate of return

In many countries, corporate income is subject to taxation. In Denmark, the corporate income tax rate is 22% [13]. Biogas installations depreciation is straight-line, this means that the value of an asset is assumed to decrease equally each year. Since the lifetime is 20 years and assuming that at the end of the project the asset value is zero the depreciation factor is 5%. Inflation also needs to be taken into account. The projected inflation for 2020 and 2021 is 1.2% [14]. Finally, the minimum rate of return also called discount rate (noted *r*) indicates the required rate of return by the investor. The higher the risk of a project the higher the discount rate. The anaerobic digestion process is well-known, in many feasibility studies, the discount rate ranges from 5 to 8% [12,15,16], which means that the investment is safe. For biogas plants that inject biomethane into the grid the minimum rate of return is generally higher [17]. Here an established technology (biotrickling filter) is used for a new application which is biogas upgrading to biomethane, hence a discount rate of 10% was selected.

III. Mass balance flowsheets

Base case design

Table S5. List of compounds involved in the simulation of the base case design [18]

Compound	***Model formula***	PROII databanks	User-defined
Insoluble carbohydrates	$C_6H_{10}O_5$		√
Soluble carbohydrates	$C_6H_{10}O_5$		√
Innert carbohydrates	$C_6H_{10}O_5$		√
Insoluble proteins	$CH_{2.03}O_{0.6}N_{0.3}S_{0.0001}$		√
Soluble proteins	$CH_{2.03}O_{0.6}N_{0.3}S_{0.0001}$		√
Innert proteins	$CH_{2.03}O_{0.6}N_{0.3}S_{0.0001}$		√
Insoluble lipids	$C_{57}H_{104}O_6$		√
Soluble lipids	$C_{57}H_{104}O_6$		√
Innert lipids	$C_{57}H_{104}O_6$		√
LCFA	$C_{18}H_{34}O_2$	√	
Ammonia (nutrients)	NH_3	√	
Acetic acid	$C_2H_4O_2$	√	
Propionic acid	$C_3H_6O_2$	√	
Lactic acid	$C_3H_6O_3$	√	
Butyric acid	$C_4H_8O_4$	√	
Valeric acid	$C_5H_{10}O_2$	√	
Cell mass	$C_5H_7O_2N$		√
Water	H_2O	√	
Methane	CH_4	√	
Carbon dioxide	CO_2	√	
Hydrogen	H_2	√	
Sulfur hydrogen	H_2S	√	

Table S6. Mass balance for the base case scenario

Stream	UOM	S3	S4	S5	S6	S7	S8	S9	S10
Total Molar Rate	kmol/h	612.75	600.95	21.99	29.33	0.18	51.51	15.04	21.79
Total Mass Rate	kg/h	12077.29	11509.56	567.70	59.13	3.10	629.93	293.98	335.95
Temperature	C	55.00	55.00	55.00	55.00	55.00	54.91	54.91	54.91
Pressure	atm	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Total Molecular Weight		19.71	19.15	25.81	2.02	17.03	12.23	19.55	15.42
Total Molar Component Rates	kmol/h								
Insoluble carbohydrates		1.31	0	0	0	0	0	0	0
Soluble carbohydrates		1.71	0.01	0	0	0	0	0	0
Innert carbohydrate fraction		0.18	0.37	0	0	0	0	0	0
Insoluble proteins		5.86	0	0	0	0	0	0	0
Soluble proteins		0.49	0.03	0	0	0	0	0	0
Innert protein fraction		0	0.88	0	0	0	0	0	0
Insolule lipids		0.03	0	0	0	0	0	0	0
Soluble lipids		0.31	0.03	0	0	0	0	0	0
Innert lipid fraction		0	0.01	0	0	0	0	0	0
LCFA		0.16	0.00	0	0	0	0	0	0
Ammonia		1.43	1.78	0	0	0.18	0.18	0.00	0
Acetic acid		1.20	10.14	0	0	0	0	0.15	0
Propionic acid		0.27	0.01	0	0	0	0	0	0
Lactic acid		0.34	0.00	0	0	0	0	0	0
Butyric acid		0.13	0.01	0	0	0	0	0	0
Valeric acid		0.06	0.00	0	0	0	0	0	0
Biomass		0.01	1.30	0	0	0	0	0.18	0
Water		596.28	585.02	0	0	0	0	14.71	0
Methane		0	0	14.31	0	0	14.31	0	20.81
CO2		2.98	1.36	7.68	0	0	7.68	0	0
H2		0	0	0	29.33	0	29.33	0	0.97
H2S		0	0	0.01	0	0	0.01	0	0.01

250,000 tonnes of substrate capacity

Table S7. Mass balance for scenario 3

Stream	UOM	S3	S4	S5	S6	S7	S8	S9	S10
Total Molar Rate	kmol/h	1531.86	1502.36	54.98	72.61	0.44	128.03	37.59	53.74
Total Mass Rate	kg/h	30193.24	28773.91	1419.25	146.37	7.58	1573.19	734.77	838.42
Temperature	C	55.00	55.00	55.00	55.00	55.00	54.91	54.91	54.91
Pressure	atm	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Total Molecular Weight		19.71	19.15	25.81	2.02	17.03	12.29	19.55	15.60
Total Molar Component Rates	kmol/h								
Insoluble carbohydrates		3.28	0	0	0	0	0	0	0
Soluble carbohydrates		4.27	0.04	0	0	0	0	0	0
Innert carbohydrate fraction		0.44	0.93	0	0	0	0	0	0
Insoluble proteins		14.65	0	0	0	0	0	0	0
Soluble proteins		1.23	0.07	0	0	0	0	0	0
Innert protein fraction		0	2.20	0	0	0	0	0	0
Insolule lipids		0.07	0	0	0	0	0	0	0
Soluble lipids		0.77	0.08	0	0	0	0	0	0
Innert lipid fraction		0	0.01	0	0	0	0	0	0
LCFA		0.39	0.01	0	0	0	0	0	0
Ammonia		3.58	4.45	0	0	0.44	0.44	0	0
Acetic acid		2.99	25.34	0	0	0	0	0.36	0
Propionic acid		0.67	0.03	0	0	0	0	0	0
Lactic acid		0.86	0.00	0	0	0	0	0	0
Butyric acid		0.34	0.02	0	0	0	0	0	0
Valeric acid		0.15	0.00	0	0	0	0	0	0
Biomass		0.03	3.25	0	0	0	0	0.44	0
Water		1490.69	1462.55	0	0	0	0	36.78	0
Methane		0	0	35.77	0	0	35.77	0	52.02
CO2		7.44	3.39	19.20	0	0	19.20	0	0
H2		0	0	0	72.61	0	72.61	0	1.711
H2S		0	0	0.014	0	0	0.01	0	0.014

IV. H2 maximum price for different *PBP*

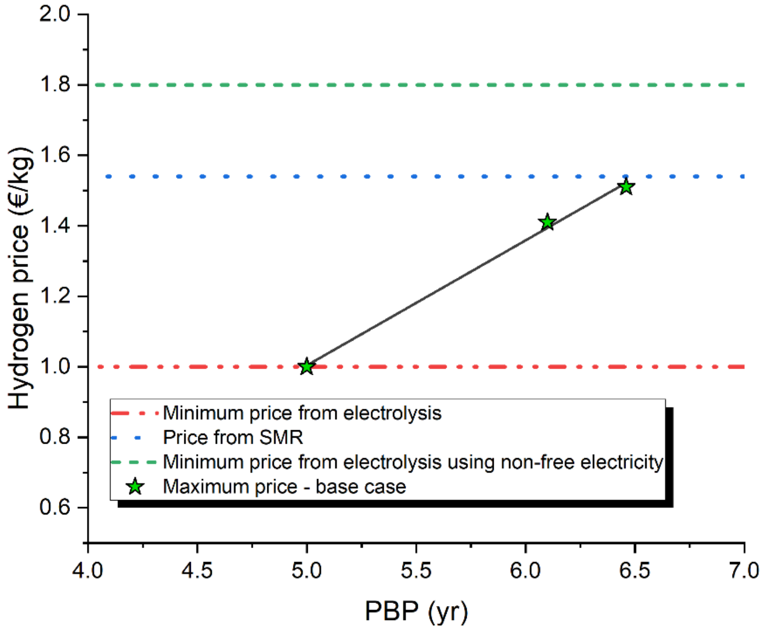

Figure S2 H_2 maximum proce estimated in this study for different *PBP* and H_2 price range from electrolysis and SMR

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