

ENHANCING BIOGAS PLANTS THROUGH POWER-TO-X INTEGRATION FOR EFFICIENT HYDROGEN AND E-FUEL PRODUCTION

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ABSTRACT

The 2023 EU targets for the green transition of hard-to-electrify sectors establish ambitious goals for renewable energy, hydrogen, e-fuels, and biomethane production, aiming to achieve unprecedented levels from 2030 to 2050. Hydrogen assumes a pivotal role in the renewable-based energy system, acting as an energy carrier for both industry and transportation sectors, and as a balancing agent for the variable nature of renewable energy sources. This paper delves into the cost-optimal design and operation of large-scale Power-to-X (PtX) hubs, emphasizing the interplay between electricity prices, grid emission intensity, and the value of behind-the-meter energy trading at the site. The analysis focuses on the GreenLab Skive PtX hub, presently under development in Denmark. The energy hub integrates multiple industries, including a large biomethane plant, a 100 MW electrolysis plant, 80 MW of renewables, with plans for methanol and other e-fuels production. For this study, we narrow our scope to hydrogen and e-methanol production, assuming the availability of a local hydrogen grid and carbon dioxide from the biomethane plant. This investigation aims to address critical questions regarding the viability of these PtX hubs, including: 1) estimation of levelized cost of hydrogen and emethanol, compliant with EU certification for renewable fuels of non-biological origin (RFNBOs), 2) identification of optimal capacity and operation of the PtX hub concerning the biogas plant's size, 3) estimation of prices for behind-the-meter trading of energy and material flow within the PtX hub and their correlation with external energy prices and CO_2 tax. The linear optimization framework Python for Power System Analysis (PyPSA) is used to model the PtX hub, identifying the combination of generation, conversion, and storage technologies that minimizes the total annualized system cost while meeting monthly production targets. Optimization variables, including capacities and power flows, are calculated with hourly resolution. The model relies on cost assumptions from the latest technology catalog by the Danish Energy Agency (2023) and constraints representing the latest EU legislation for RFNBOs (2023). Energy prices and emission intensities are based on 2022 with a sensitivity analysis on CO₂ tax. The forecasted (2030) LCoE for hydrogen is estimated at about 3 (€/kg), with a plant operating approximately 4000 hours per year at full load capacity, and around 4 (€/kg) if renewable electricity from the grid complements existing on-site renewables. E-methanol production, facilitated by the scale difference between the biogas plant and large-scale hydrogen production, incurs a LCoE of about 750 (€/t_{MeOH}), aligning with the price of fossil methanol when a CO₂ tax of approximately 180 (ϵ/t_{CO2}) is applied. E-methanol costs rise rapidly if CO₂ recovery from biogas upgrading exceeds 85%, necessitating intermediate storage; hence, full CO2 recovery is not advised.

1 INTRODUCTION

The current European strategy for green transition arises from the confluence of stringent sustainability targets and the geopolitical instability stemming from the Ukraine-Russia crisis. These dual imperatives have compelled the European Commission (EC) to undertake a substantial revision of EU strategy for the green transition, initially with the Fit for 55 package and afterwards with the more ambitious REPower EU plan [1]. The combination of these measures is fostering the renewables while diminishing the European Union's dependency on imported hydrocarbon resources. On one hand, the Fit for 55 targets aim to a 30 percent reduction in gas consumption by 2030, consequently mitigating the need for imports of hydrocarbon-based resources. On the other hand, the introduction of REPowerEU plan leads to more advanced and ambitious targets pertaining to renewable energy and renewable fuels (Commission, 2022), in particular enhancing the production of hydrogen, e-fuels and biomethane to unprecedented levels.

Hydrogen will have a pivotal role in the renewable-based energy system envisioned by the REPowerEU plan, serving both as energy carrier for industry and transportation sectors and as balancing agent for the variable nature of renewable energy sources (RE). The REPowerEU plan clearly indicates a target of 10Mt/y (European Commission, 2020) for hydrogen production in EU by 2030, which will accommodate the demand for industry sector and production of electro-fuels for shipping and aviation and fertilizers (European Commission, 2020). The targets are set considering the extensive electrification of transport sector and residential heating. Meeting the demand for hydrogen necessitates an expansion of RES and the extensive integration of Power-to-X (PtX) technologies, with an anticipated 65 GW of hydrogen production capacity from installed electrolysis units in the EU by 2030. However, it is imperative that the power driving PtX processes is of renewable origin to ensure alignment with the overarching objective of transitioning away from fossil fuels. The electricity used in PtX must either be sourced from surplus renewable energy, where the PtX system aids in grid balancing, or from a dedicated renewable power source adhering to the additionality principle (European Commission, 2023b) (European Commission, 2023a). Among off-takers of renewable hydrogen the e-fuels production is a primary driver, particularly for decarbonizing significant markets such as marine shipping and aviation [5]. Renewable methanol stands out for its versatility, finding applications as a shipping fuel, chemical feedstock, and intermediate chemical for kerosene synthesis. Carbon sources for synthesis of Renewable Fuels of Non-Biological Origin (RNFBOs) should also be biogenic to reach the set threshold of minimum 70% GHG reduction compared to the fossil counterpart. Co-location of renewable carbon resources and high-RES areas is a desirable condition, as it obviates the need for hydrogen or power transport, along with their associated costs and potential grid balancing issues. However, the geographical placement of biogenic carbon sources is often dictated by factors such as transport costs for biomass (e.g. biogas plants) and proximity to end-users (e.g. biomass-fired and waste incineration plants).

A pathway offering a unique solution to these specific challenges is the integration of PtX hubs with biomethane plants which, are frequently situated in rural areas endowed with abundant RES, exemplified by Denmark and northern Germany. E-fuels in such PtX hub is limited to medium scale by the availability of biogenic CO_2 and these plants are less likely to impose additional strain on the existing power grid and more likely to leverage curtailed power to locally balance the grid. While hydrogen infrastructure is not a prerequisite for e-fuel production, it can enhance productivity, making it a desirable addition. An additional drive for e-fuel synthesis at biomethane plants stems from their potential for CO_2 neutrality (European commission, 2023c), when utilizing CO_2 derived from biogas production processes, specifically wet manure from closed digestate production.

The ambition of this investigation is to provide an in-depth cost estimation of hydrogen and e-methanol produced in such PtX hubs integrated with biomethane plants, and to complement the existing literature on cost estimation for renewable hydrogen and e-fuels (IEA, 2023) (IRENA & Methanol institute, 2021) (Neumann et al., 2023) (Kountouris et al., 2023) (Mortensen et al., 2020). This paper is grounded on the analysis of one of first large-scale commercial projects of this kind the GreenLab Skive (GLS), located in the northern region of Denmark. In 2021, the Danish government designated GreenLab as an official regulatory test zone granting GreenLab the opportunity to balance behind-the-meter trading of

renewable electricity (RE) and other energy and material flows. The test zone permit is one of a kind in Europe, providing valuable insights for all of Europe's green transition. The PtX concept at GLS primarily revolves around the conversion of local biogenic waste via in the existing large-scale biogas plant and hydrogen production based on the on-site renewables. This platform provides an opportunity for other up-takers of hydrogen, CO_2 and to join the PtX hub for production of other commodities as e-methanol synthesis but it is not limited to energy-related industries. Comparable PtX hubs are anticipated to emerge in other locations as well. In this study only MeOH via CO_2 hydrogenation is considered other processes are suitable as production based on reforming of biogas (Rinaldi et al., 2023), which is not presently considered as primary pathway for e-fuels due to the high market value of biomethane as a natural gas substitute.

This investigation aims to address several critical questions about the viability of this type of PtX hubs: 1) estimation of levelized cost of energy (LCoE) for hydrogen and e-methanol, compliant with EU certification for renewable fuels of non-biological origin (RFNBOs), 2) identification of optimal capacity and operation of the PtX hub concerning the biogas plant's size, 3) estimation of prices for behind-the-meter trading of energy and material flow within the PtX hub and their correlation with external energy prices and CO_2 tax. The production of MeOH is compared in two configurations: integrated with the H₂ production for the grid and a standalone. The integrated configuration benefits from lower cost for the electrolyzer and sharing of local hydrogen infrastructure, hence the results can give an indication of the value of H_2 pipelines for this type of business. To address these questions, we utilize the open capacity expansion model Python for Power System Analysis (Brown et al., 2018) (PyPSA), which is here applied to characterize the industrial stakeholders in the PtX hub. The model co-optimizes the investment for generation, conversion, storage, and distribution of the main energy and material flows to achieve the least-cost outcome. Unlike other techno-economic studies (Lacerda de Oliveira Campos et al., 2022; Mbatha et al., 2021) (Marlin et al., 2018) (Nemmour et al., 2023) (Nieminen et al., 2019) (Pratschner et al., 2023) (Sollai et al., 2023) (Sorrenti et al., 2023), our aim here is to capture the dynamic interactions in the energy hub, both internally and with the broader energy systems. Presently, the estimated costs for renewable hydrogen range from 3 to 12 €/kg (IEA, 2023; IRENA, 2023), a range primarily influenced by the capital costs of electrolyzers and the levelized cost of renewable electricity. The estimated production cost for e-methanol highly influenced by the cost for renewable hydrogen and carbon. The current cost the range is estimated in 750 to 1500 (€/t) (Methanol Institute, 2022) and as compared to 350-500 (\notin /t) of fossil methanol.

2 METHODOLOGY

2.1 Overall approach

The cost analysis for hydrogen and e-methanol production within the integrated PtX hub was conducted using the PyPSA linear optimization model, as introduced in (Brown et al., 2018). In this study, PyPSA is employed to identify the most efficient combination of generation, conversion, and storage technologies within the integrated PtX hub. This combination minimizes the total annualized system cost while ensuring a consistent supply of energy and materials flows to meet demands. The optimization variables encompass the capacities and power flows of each technology, calculated with 1 hourly time resolution. For the optimization, we set the annual demands for hydrogen and methanol, in addition to the fixed demand and capacity for the biomethane plant. The external energy system is represented by an interface described in Table 1, facilitating the import or export of electricity, natural gas. The spot prices for external are assumed to be inelastic, not accounting for supply or demand responses related to the operation of the PtX hub. Two years of reference have been used in this study for energy prices (electricity and NG) and emissions intensities: 2019 and 2022. These two years have manifested significantly different prices with low figures in 2019 and high prices in 2022 due to the Ukraine-Russia crisis. The trading of electricity between the grid and the PtX hub is facilitated through the application of purchasing and selling prices at the interface, where hourly purchasing prices for each scenario $(p_{el,t}^{in,SC})$ are calculated as the sum of spot price $(p_{el,t}^{ref})$, all the purchasing tariffs (TF_p) for TSO, DSO and state (in DK1 area) level and CO₂ tax (p_{CO2}^{SC}) times the emission intensity (em_l) .

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	H ₂ production for Grid	CO ₂ recovery to MeOH	CO ₂ cost (€/ton)	Energy prices year	Biomethane production	MeOH production
SC1	272 (GWh/y)	0.7 - 0.99	150	2019	190 (GWh/y)	Integrated
SC2	272 (GWh/y)	0.7 - 0.99	150	2022	190 (GWh/y)	Integrated
SC3	0	0.7 - 0.99	150	2019	190 (GWh/y)	Stand-alone
SC4	0	0.7 - 0.99	150	2022	190 (GWh/y)	Stand-alone

Table 1: reference scenarios for the optimization of GLS PtX hub

Selling price to the grid are set equal to the spot price. Similar approach is followed for the purchase of natural gas. Tariffs for electricity in Demark (DK1 area) are summarized in table 2. For the scope of this investigation, we set an overall CO₂ tax for fossil emission from grids electricity and natural gas equal 150 ((ϵ/t_{CO2})). Constraints are imposed on the use of grid electricity for hydrogen and e-methanol production according to the RFNBOs legislation (European Commission, 2023b) as the electricity supplied to both the hydrogen and MeOH production (including compression of gases) must be renewable or can be purchased from the grid if the electricity price is below 20 ((ϵ/MWh)), via equation 12. Four scenarios were defined and are shown in Table 1 defined by the energy year (2019 or 2022) and the hydrogen demand to the grid set to 272 (GWh/y) corresponding to about 4000 full load hours for a 100MW plant, or zero for standalone MeOH production. The scenarios are parametrized for the MeOH demand expressed by the rate of CO₂ recovery form the biomethane upgrading with the highly variable renewables and H₂ production may require considerable investments in storage of CO₂ or hydrogen. Hence, identifying what CO₂ recovery rates are acceptable was relevant for all scenarios.

2.2 PyPSA model of the PtX hub

The model operates under the assumption of an ideal market characterized by perfect competition among all featured technologies and the maintenance of long-term market stability hence, all energy technologies recuperate exactly their entire costs. The Lagrange multiplier, also known as Karush-Kuhn-Tucker (KKT), is associated for every hour t with the demand constraint indicating the marginal price of the energy carrier in the bus. The KKT multipliers for demand constraints of hydrogen and methanol were here interpreted as LCoE for those carriers. Lagrange multipliers for internal buses were instead represent equilibrium prices for the behind-the-meter trading at the PtX hub e.g. local marginal price for the internal electricity or CO_2 buses. The power capacity of conversion technologies (links) is not explicitly constrained in the formulation of the optimization problem, except for the original biomethane plant, which serves as a reference. No investment cost is associated with the biomethane plant, and only operational cost differences are considered. Additionally, the model assumes a level of foresight that enables precise anticipation of energy supply and demand throughout the year. This includes accounting for year-ahead weather forecasts, energy prices, and emission intensities of external energy systems. As a result, any form of storage intended as a precaution against unforeseen energy shortages is not considered in this model. PyPSA is an open-source toolkit dedicated to simulating and optimizing modern power and energy systems. It encompasses a spectrum of functionalities and components which are extensively described of the official documentation. The mathematical formulation of PtX hub used in this study model is summarized by equations 1-12 and the model is available on Github. In the formulation the index s indicates dispatchable generators, t indicated the time steps, n indicated buses (enforcing energy conservation), and l is the index for links. The optimization objective is the total annualized systems cost formulated as in Eq.1 in table A.1. Where $G_{n,s}$ is the power capacity of generators and $c_{n,s}$ are the associated fixed annualized costs. $E_{n,s}$ and $\hat{c}_{n,s}$ are the energy store capacity and its associated fixed annualized cost and F_{l} and c_{l} are the power capacity and associated annualized cost for connecting link *l*. The objective function is completed by the variable costs $o_{n,s,t}$ for generation $g_{n,s,t}$ and the variable cost $o_{l,t}$ for dispatch $f_{l,t}$ trough links, at every hour t. The optimization is subject to a list of linear equality and inequality constraints. Eq.2 reports the constraint for energy conservation at each bus n, where hourly demand $d_{n,t}$ must be supplied by generators or imported from other buses via links.

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Commodity	Price model		
Electricity purchased from the grid	$p_{el,t}^{in,SC} = p_{el,t}^{\mathcal{Y}} + TF_p + em_t \cdot p_{CO2}^{SC}$		
Electricity sold to the grid	$p_{el,t}^{out,SC} = p_{el,t}^{\mathcal{Y}}$		
Natural gas purchased from the grid	$p_{NG,t}^{in,SC}=p_{NG,t}^{\mathcal{Y}}+em_{NG}~\cdot p_{CO2}^{SC}$		
Total tariffs on electricity purchase	120 – 124 (€/MWh) in DK1 area		

Table 2: Prices for trading of electricity and natural gas between the external grids and the PtX hub

The energy flow of link $(f_{i,t})$ is multiplied by efficiency coefficient $\alpha_{n,t}$ indicating both the direction and the efficiency of the flow between the buses connected by the multilink. The equality constraint expressed by Eq.2 are associated with the Lagrange multiplier $\lambda_{n,t}$, also known as Karush-Kuhn-Tucker (KKT), indicating the marginal price of the energy carrier in the bus. The power dispatched by generators is constrained for every hour (Eq. 3) by the product of the between the installed capacity $G_{n,s}$ and the minimum and maximum availabilities $\underline{g}_{n,s,t}$ and $\overline{g}_{n,s,t}$. For renewables the minimum availability is zero and the maximum availability is the capacity factor at time t. The power capacity of all generators can be limited by the potential \overline{G}_s related to physical and environmental constraints (Eq. 4), however in this formulation of the optimization problem the power capacity of generators and links were not constrained, except for the fixed capacity of the biomethane plant. Inequality constraints for links are described by Eqs 5 and 6. The maximum power flowing through the links is limited by their maximum physical capacity F. For bidirectional transmission links, $f_{l,t}$ and $\overline{f}_{l,t}$ are equal respectively to -1 and 1. For energy conversion processes (unidirectional) $f_{l,t}$ and $\overline{f}_{l,t}$ are equal respectivlely to 0 and 1. The power capacity of all links can be limited by the potential (\overline{F}_l) related to physical and environmental constraints (Eq.6), for example the charging and discharging of stores is controlled by links limiting the maximum power and setting the efficiencies ($\alpha_{n,l,t}$).

$$\min_{\substack{G_{n,s}, E_{n,s}, \\ g_{n,s,t}, g_{n,l,t}}} \sum_{\substack{E_{n,s}, F_l}} \sum_{n,s} c_{n,s} \cdot G_{n,s} + \sum_{n,s,t} \hat{c}_{n,s,t} \cdot E_{n,s,t} + \sum_{l} c_l \cdot F_l + \sum_{n,s,t} o_{n,s,t} \cdot g_{n,s,t} + \sum_{l,t} o_{l,t} \cdot f_{l,t}]$$
(1)

Subject to:

$$\sum_{s} g_{n,s,t} + \sum_{l} \alpha_{n,l,t} \cdot f_{l,t} = d_{n,t} \quad \leftrightarrow \lambda_{n,t} \quad \forall n,t$$
⁽²⁾

$$g_{n,s,t} \cdot G_{n,s} \leq g_{n,s,t} \leq \overline{g}_{n,s,t} \cdot G_{n,s} \quad \forall \ n,s,t$$
(3)

 $0 \le G_s \le \overline{G}_s \quad \leftrightarrow \ \mu_s \quad \forall \ s \tag{4}$

$$f_{l,t} \cdot F_l \le f_{l,t} \le \overline{f}_{l,t} \cdot F_l \quad \forall \, l,t \tag{5}$$

$$0 \le F_l \le \overline{F}_l \iff \mu_l \quad \forall l \tag{6}$$

$$0 \le e_{n,st,t} \le E_{n,st} \quad \forall \, n, st, t \tag{7}$$

$$0 \le E_{st} \le \overline{E}_{st} \leftrightarrow \mu_{st} \quad \forall st \tag{8}$$

$$-g_{dw,s} \le g_{s,t} - g_{s,t-1} \le g_{up,s} \quad \forall s,t$$

$$\tag{9}$$

$$-f_{dw,l} \le f_{l,t} - f_{l,t-1} \le f_{up,l} \quad \forall \, l,t \tag{10}$$

$$\overline{f}_{gridtoH2,t} = 1 \quad \forall \ t, \ el_{price,t} \le 20 \ \left(\frac{\notin}{MWh}\right) \tag{11}$$

$$\sum_{t} d_{elDK1,t} = \left(\frac{\sum_{t} d_{H2,t}}{\alpha_{H2/el}} + \frac{\sum_{t} d_{MeOH,t}}{\alpha_{MeOH/el}} \right) \cdot 0.1$$
⁽¹²⁾

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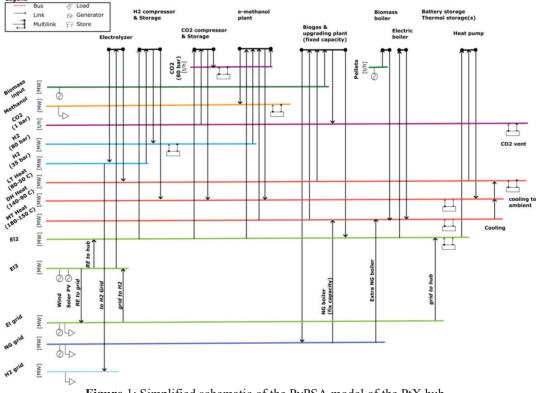


Figure 1: Simplified schematic of the PyPSA model of the PtX hub

The energy content of a store $e_{n,st,t}$ is constrained by the installed energy capacity $E_{n,st}$ (Eq. 7). The energy capacity of a store can be limited by other physical and environmental constraints (Eq. 8), e.g. the maximum allowed H₂ storage depends on the legal permitting at the site. Other additional technical constraints are the ramp-up and ramp down for generation and energy conversion technologies. These constraints are described in Eqs. 9 and 10 where the difference in generated or converted power between one snapshot and the other is limited by lower ($gdw_{s,t}$ and $fdw_{s,t}$) and higher ($gup_{s,t}$ and $fup_{s,t}$) bounds. The costs and estimated lifetimes of all technologies are presented in Table 4 with the matching references. Cost assumptions in this study are largely based on the Technology catalogue from the Danish Energy Agency (DEA) (Danish Energy Agency, 2023), which provides with performance and cost assumptions and forecast for the upcoming years. Investment year 2030 was selected to provide a reliable cost estimation for the forthcoming development of the hydrogen and e-fuel economy, thus minimizing uncertainties in cost projections. Investment expenses are amortized over the reported lifespan of each asset, considering a discount rate of 7%. On-site storage of liquid MeOH was assumed available and the production was optimized independently of the actual delivery to the market.

A graphical representation of the model is shown in Figure 1. The representation omits several details in the model and a full-scale graphical representation is available on Github. On the left-hand side of Figure 1, the buses forming part of the external grids (El1, NG, and DH) are displayed. Within the PtX Hub, two electricity buses have been identified. The first (El3) connects RE (wind and solar) generation and hydrogen production, while the second (El2) links all other loads, which do not necessarily require RE sources. These two electricity buses are connected by a link (RE to hub) and are independently linked to the external grids for electricity and natural gas are modelled applying the 2019 and 2022 demands for the respective market areas with generators able to satisfy them without adding any cost to the objective function. The trading of electricity between the grid and the PtX hub is facilitated through the application of purchasing and selling prices to the links: *grid to hub, grid to H2*, and *RE to grid* (Fig. 2), with different taxes and tariffs for sale and purchase (Table 1). The sales of renewable

electricity from GLS to the external grid is subject to the demand of the external grid demand which is scaled from the timeseries of the actual electricity demand in DK1 area.

Technology	Reference flow	Investment cost	Fixed O&M cost	Variable O&M cost	Lifetime
		(k€/ ref.)	(%/y)	(€/MWh _{ref})	(y)
On-shore wind	Electricity (MW)	1040	1.22	1.35	30
Solar PV	Electricity (MW)	380	1.95	-	40
Grid connection	Electricity (MW)	140	2	-	40
Electrolysis (100 MW)	Electricity (MW)	575	4	-	25
Electrolysis (10 MW)	Electricity (MW)	900	4	-	25
Water purification	Water (t/h)	135	2	-	25
NG boiler	Heat (MW)	50	1.04	1	20
Electric Boiler	Heat (MW)	70	1.0	1.0	25
Biomass boiler	Heat (MW)	590	7.5	-	20
MeOH Synthesis	Methanol (MW)	651	3.0	-	30
CO ₂ compressor	$CO_2(t/h)$	1516	4.0	-	15
H ₂ compressor	$H_2(MW)$	79.4	4.0	-	15
CO ₂ liquefaction	CO ₂ (t/h)	19.76	5.0	-	25
CO2 storage	$CO_2(t)$	2.53	1.0	-	25
H ₂ vessel	H ₂ (MWh)	12.3	2.0	-	20
Transformer	Electricity (MW)	0.140	2.0	-	40
Li-ion battery	Electricity (MWh)	0.142	-	-	25
Battery inverter	Electricity (MW)	0.160	0.34	-	10
Hot water tank	Heat (MWh)	0.540	0.55	-	25
Thermal battery	Heat (MWh)	25	-	-	25
Heat network	Heat·km (MW·km)	25	-	-	25
Heat exchangers	Heat	100	-	-	25
Local H ₂ pipe	H ₂ ·km (MW·km)	3.8	3.17	-	50
Local CO ₂ pipe	CO ₂ ·km (t/h·km)	130	0.1	-	50
Heat pumps	Heat (MW)	780	0.11	3.2	20

Table 4: main cost assumptions for year 2030.

The scaling of the external electricity demand is necessary to prevent solutions which excessively favor sales of RE from the PtX hub in favorable market condition hence, to keep the research focus on RFNBOs production. The external annual external electricity demand is set proportionally to a simple estimation of the yearly electricity consumption for RFNBO production (eq.12), assuming that sales to the external grid can be up to the 10% of the estimate. The purchase of electricity from the grid for RFNBOs production is constrained by equations 11, which applies on the link grid to H2 with hourly resolution (matching RFNBOs regulation for post-2030 period). The cost for the electrical infrastructure at GLS is roughly estimated by the cost of transformers and connection to the external distribution grid (60kV) (Danish Energy Agency, 2023). Only alkaline electrolysis is considered in this study, with different investment cost for grid application 575 (€/MW) and standalone plant 575 (€/MW) according to [19]. Hydrogen is produced at 35 bars and distributed to the methanol synthesis section where pressure is increased to 80 bar, the work required for compression is estimated into 0.34 (MWh/t_{H2}) (Atsonios et al., 2016) (Sollai et al., 2023). Hydrogen can be stored in steel vessels (Danish Energy Agency, 2023), with an additional work required of 0.06 (MWh/t_{H2}). Methanol synthesis is not a process which offers flexibility towards intermitted operation as temperature and pressure conditions must be maintained throughout the whole process for efficient and safe operation. Hence, storage of CO₂ and/or H₂ is required for coupling with intermittent energy sources. Capacity and operation of hydrogen and CO₂ compressors and storages are optimized separately from the MeOH synthesis process. Cost inputs and mass and energy balances for methanol synthesis via CO₂ hydrogenation refer to the DAE catalogue and have been complemented with other sources (Nieminen et al., 2019) (Pratschner et al., 2023) (Esteban & Romeo, 2021) (Kountouris et al., 2023). Constraints for ramp-up and -down are set in the model equal to 48h for increasing production from zero to full capacity, or vice

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versa. Carbon dioxide is obtained from the biomethane upgrading at atmospheric pressure and requires compression to 80 bars with work of 0.096 (MWh/t_{CO2}). Storage of liquefied CO₂ is included in the model according to (Danish Energy Agency, 2023). The biogas plant is designed to process up to 500 000 tons per year of animal manure and residual products from agriculture and food industry. The plant is usually operated to process 300 000 tons per year sources in the neighbor regions corresponding to a production of about 200 (GWh/y) of biomethane. Biogas is upgraded to biomethane trough an amine scrubber which required 0.085 MW of heat for each MW of biomethane currently obtained through combustion of natural gas. The product biomethane is compressed to the grid pressure of 40 bar for injection. As aforementioned, no capital costs are associated to the standard operation of the Skive Biogas plant and all the investments, including the NG boiler are considered sunk costs. Sales of biomethane are not included in the objective function as the capacity and operation of the biomethane plant are fixed. However, purchase of NG from the grid is included in the objective function, with NG prices adjusted for CO_2 tax (table 2). The model of the heat network in GLS can operate on three temperature levels (Figure 1): 1) pressurized hot water with temperature in the range 180-150 °C (MT heat), 2) pressurized hot water for temperature 150 - 90 °C (suitable for district heating), and 3) hot water in between 90 and 50 °C (LT heat). The three networks satisfy specific demands the medium temperature network supplies heat to the amine scrubber and the methanol distillation, a heat pump system is available for upgrading of LT heat to DH temperature, inputs are based on (Danish Energy Agency, 2023). However, connection to an external DH grid is not included in this study. Storages of heat is possible with two technologies: a thermal battery operating at temperatures as high as 350 °C using electricity and a hot water tank for storage at about 95 °C. Input data for the thermal battery refer to commercial concrete-based technology (Hoivik et al., 2019). The cost for the heat network infrastructure was estimated using an guesstimate of the piping length of km and a cost for all the heat exchangers (Danish Energy Agency, 2023). In addition to the existing natural gas boiler three other technologies for heat production are considered in the model: biomass boiler using straw pellets from digestate fibers, electric boiler, and an additional natural boiler. Other modelling assumptions as heat demands for each single plant can be obtained from the Github repository.

3 RESULTS AND DISCUSSION

Prices for behind the meter trading are obtained from the KKT multipliers on the respective buses of the model, for all the energy and material streams. For products with exogenously set demand the KKT multiplier represents the LCoE in the optimal solution. Simultaneously the capacity of all the components and their operation are optimized. KKT multipliers and total annualized system cost are the main indicator used in the results for evaluating the four scenarios presented in table 1.

3.1 Methanol production

The production of Methanol in the PtX hub is significantly influenced by two factors the fraction of CO₂ recovered to MeOH and the integration with a larger hydrogen production plant. Figure 2 reports the KKT multiplier for MeOH as function of the carbon form biomethane upgrading recovered in the MeOH and parametrized for the demand of the H₂ to the grid, hence comparing integrated plants and standalone MeOH plants, the latter baring higher costs for electrolysis. The impact of the other external energy prices is minimum as the system runs essentially on on-site renewable resources. It is evident as the LCoE for MeOH is considerably lower for the integrated MeOH solution which can benefit from the existing infrastructure for hydrogen production and the hydrogen grid to reduce costs for storage and compressors compared to the standalone solution. Recovering all the CO₂ available from the biomethane upgrading significantly increases LCoE for methanol due to increased storage capacity (H₂ and/or CO_2) required to balance the steady operation of biomethane upgrading and the intermittent operation of renewables. For an integrated plant is feasible to recover up to 95% of the carbon in the separated CO₂ without excessively increase costs, instead maximum 85% is advised for standalone plants. The production cost is estimated in 740-765 (€/t) for integrated MeOH production and 850-870 (\mathbf{E}/\mathbf{t}) for standalone plants with high risk of increasing production cost is carbon recovery is enhanced in the latter case.

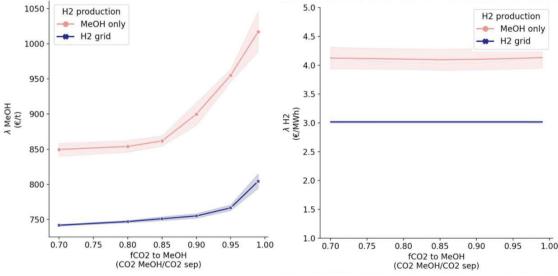


Figure 2 – LCoE for MeOH and hydrogen

For comparison fossil methanol (priced at $360 \notin t$) would require a CO₂ tax of 180 ($\notin t_{CO2}$) to reach a similar market price with estimated life cycle emissions of 110 g/MJ (IRENA & Methanol institute, 2021).

3.2 Hydrogen production and GLS behind-the-meter market

Hydrogen production is evaluated together with the rest of the behind-the meter market for energy and material streams in figure 3. The figure shows the yearly distribution of KKT multipliers for behindthe-meter trading and on the right the energy prices external in external grids. All the prices are reported in (\notin /MWh) except for CO₂ (\notin /t). The LCoE for hydrogen is around 3 (\notin /kg) for grid scale production and 4 (\mathcal{E} /kg) for local production for MeOH. The LCoE of H₂ is not related to the energy prices in the grid under current modelling setup with additionally principle for RFNBOs and use of grid electricity only below 20 (€/MWh). This is not the case for the other commodities traded within GLS. Electricity prices are correlated to the external grid prices, however maintaining average price well below the grid price thanks to the on-site renewables. On average behind-the-meter electricity price is 25 - 40% of the grid purchasing price depending on the scenarios. The price for CO_2 from the biomethane upgrading is generally low (0-10 \in /t) compared to the CO₂ tax and rises with CO₂ recovery rate to MeOH, hence it correlates strongly with MeOH cost. The price for MT heat is around 8-10 (€/MWh) considerably low that NG price with CO₂ tax due heat integration among the plants and use of biomass and renewable electricity. Other plants in the PtX hub can benefit from the lower energy prices as biomethane which shows reduction in production cost of 15 -28 (\notin /MWh_{CH4}). The annualized total system cost is highly dependable on demand for hydrogen grid as it drives both investment to the electrolysis and renewables. Figure 3 on the left, shows the total system cost and the breakdown of capital costs. Renewables and electrolysis account to for more than 95% of the annualized investment cost, with a minor investment in MeOH synthesis (including compressors and storages of H_2 and CO_2). It is worth reminding here that at the optimal solution the total cost of each component, hence of the system, is fully recovered if the exogenous demands (H₂ and MeOH) are traded to external grids, at their KKT multiplier. The righthand side of figure 3 reports the size of the four largest components in the system by investment cost. For grid scale application about 120 (MWel) of electrolysis are required with about 240 (MWel) of onshore wind and 40 (MWel) of solar. The standalone MeOH system has a smaller size with 25 (MWel) of electrolysis supported by 50 (MW_{el}) of wind and 20 (MW_{el}) of solar. The capacity of the MeOH synthesis plant is lower in the grid scale scenarios (8 MW_{MeOH}) than the standalone scenarios (13.5 MW_{MeOH}) despite the higher recovery rate of CO₂, due to a more continuous operation of the MeOH plant and lower storage capacity installed.

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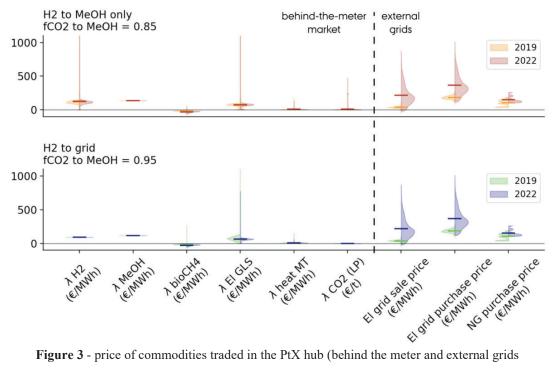


Figure 3 - price of commodities traded in the PtX hub (behind the meter and external grids

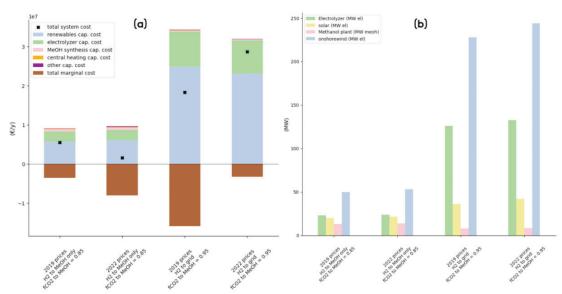


Figure 4 (a, b): a) system cost break-down, b) Optimal capacity of main components

4 **CONCLUSIONS**

Integration of large electrolysis plants with biogas plants provides a solid platform for synthesis of efuels synthesis potentially reducing LCoE of products, increasing utilization of the plants, reducing need for storage and benefitting other plant located in the PtX hub. LCoE for MeOH integrated with large scale H₂ production is estimated around 750 ((ϵ/t)) with CO₂ recovery rate up to 95% and 850 ((ϵ/t)) with CO_2 recovery rate up to 85% for standalone plants. Increasing CO_2 recovery rate corresponds to

significant increase in LCoE. For comparison fossil methanol (priced at 360 €/t) would require a CO₂ tax of $180 \text{ (€/t}_{CO2})$ to reach a similar market price. The behind-the-meter market consistently provides electricity and heat prices lower than the external grids. The investment costs in the renewables and electrolysis plant, accounting for 95% or more of the total investment cost for both integrated and standalone MeOH production.

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DATA AND CODE AVAILABILITY

The code to reproduce the results and visualizations is available on GitHub (https://github.com/BertoGBG/GLS_greenbubble), together with all input. Technology data assumptions were taken from github.com/pypsa/technology-data (v0.4.0). We also refer to the documentation of PyPSA (pypsa.readthedocs.io), for technical instructions on how to install and run the model.

NOMENCLATURE

Subscripts		Superscripts			
t	Dispatching periods	ref	reference year		
S	Generators	SC	scenario		
n	Buses	in	purchase		
ld	Loads	out	sales		
l	Links				
st	Stores				
Parameters			(* ***** M ·)		
fCO ₂ MeOH	Fraction of CO ₂ from biomethane upg	(MW/h)			
Variables					
G_s	Power capacity of technology (s)		(MW)		
C _s	Fix annualized costs for power capaci	(€/MW)			
E_s	Store Energy capacity of technology ((MWh)		
Ĉ _s	Fix annualized costs for power capaci	(€/MWh)			
$g_{s,t}$	Power dispatch of technology (s) at tin	(MW)			
0 _{s,t}	Variable cost of technology (s) at time	(€/MW)			
$d_{ld,t}$	Demand of load (d) at time (t)	MW			
$\alpha_{lk,t}$	Efficiency and flow direction on the b	(MW/MW)			
f _{lk,t}	Energy or material flow for link lk at t	(MW)			
f _{lk,t}	Minimum power availability of link (MW				
$\frac{f_{lk,t}}{\overline{f}}_{lk,t}$	Maximum power availability of link	(MW/MW_{max})			
$ \frac{g_{gn,t}}{\overline{g}_{gn,t}} \\ \frac{e_{st,t}}{\overline{g}_{\overline{l}}} \\ \frac{\overline{g}_{\overline{l}}}{\overline{g}_{\underline{l}}} $	Minimum power availability of genera	(MW/MW_{max})			
$\overline{g}_{gn,t}$	Maximum power availability of gener	ator	(MW/MW_{max})		
e _{st,t}	Energy level in a storage (st) at time t	(MWh)			
$\overline{g_1}$	Ramp-up power constraint for dispate	(MW/h)			
\overline{g}_{l}	Ramp-down power constraint for disp	(MW/h)			
$\lambda_{n,t}$	KKT multiplier for energy balance at	(€/MW)			
μ	KKT multiplier for inequality constrain	(€/MWh)			
$p_{el,p,t}$	Total electricity price for purchase fro	(€/MWh)			
$p_{elREF,t}$	Spot price for electricity during the re-	(€/MWh)			
$TF_{el,p}$	Total tariff for purchase of electricity	(€/MWh)			
em_t	Emission intensity of electricity produ	(tCO ₂ /MWh)			
p_{CO2}	CO2 tax (dependent on scenario)		(2)		
1 002					

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REFERENCES

- Atsonios, K., Panopoulos, K. D., & Kakaras, E. (2016). Investigation of technical and economic aspects for methanol production through CO2 hydrogenation. *International Journal of Hydrogen Energy*, 41(4), 2202-2214.
- Brown, T., Hörsch, J., & Schlachtberger, D. (2018). PyPSA: Python for Power System Analysis. *Journal of Open Research Software*.
- Supplementary to Directive (EU) 2018/2001 rules on renewable e-fuels, (2022).
- Danish Energy Agency. (2023). Technology Data. In.
- Esteban, M., & Romeo, L. M. (2021). Techno-Economics Optimization of H2 and CO2 Compression for Renewable Energy Storage and Power-to-Gas Applications. *Applied Sciences*, 11(22), 10741.
- European Commission. (2020). A hydrogen strategy for a climate-neutral Europe.
- European Commission. (2023a). Delegated Regulation 2023/1184.
- European Commission. (2023b). Delegated regulation 2023/1185.
- European commission. (2023c). Renewable Energy Directive EU/2023/2413.
- Hoivik, N., Greiner, C., Barragan, J., Iniesta, A. C., Skeie, G., Bergan, P., Blanco-Rodriguez, P., & Calvet, N. (2019). Long-term performance results of concrete-based modular thermal energy storage system. *Journal of Energy Storage*, 24, 100735.
- IEA. (2023). Global Hydrogen Review.
- IRENA. (2023). Renewable power generation costs in 2022.
- IRENA, & Methanol institute. (2021). *Innovation Outlook : Renewable Methanol*. International Renewable Energy Agency.
- Kountouris, I., Langer, L., Bramstoft, R., Münster, M., & Keles, D. (2023). Power-to-X in energy hubs: A Danish case study of renewable fuel production. *Energy Policy*, 175, 113439.
- Lacerda de Oliveira Campos, B., John, K., Beeskow, P., Herrera Delgado, K., Pitter, S., Dahmen, N., & Sauer, J. (2022). A Detailed Process and Techno-Economic Analysis of Methanol Synthesis from H2 and CO2 with Intermediate Condensation Steps. *Processes*, 10(8), 1535.
- Marlin, D. S., Sarron, E., & Sigurbjörnsson, Ó. (2018). Process Advantages of Direct CO2 to Methanol Synthesis [Original Research]. *Frontiers in Chemistry*, 6.
- Mbatha, S., Everson, R. C., Musyoka, N. M., Langmi, H. W., Lanzini, A., & Brilman, W. (2021). Power-tomethanol process: a review of electrolysis, methanol catalysts, kinetics, reactor designs and modelling, process integration, optimisation, and techno-economics [10.1039/D1SE00635E]. *Sustainable Energy & Fuels*, 5(14), 3490-3569.
- Methanol Institute. (2022). Carbon footprint of methanol.
- Mortensen, A. W., Mathiesen, B. V., Hansen, A. B., Pedersen, S. L., Grandal, R. D., & Wenzel, H. (2020). The role of electrification and hydrogen in breaking the biomass bottleneck of the renewable energy system – A study on the Danish energy system. *Applied Energy*, 275, 115331.
- Nemmour, A., Inayat, A., Janajreh, I., & Ghenai, C. (2023). Green hydrogen-based E-fuels (E-methane, Emethanol, E-ammonia) to support clean energy transition: A literature review. *International Journal* of Hydrogen Energy, 48(75), 29011-29033.
- Neumann, F., Zeyen, E., Victoria, M., & Brown, T. (2023). The potential role of a hydrogen network in Europe. *Joule*, 7(8), 1793-1817.
- Nieminen, H., Laari, A., & Koiranen, T. (2019). CO2 hydrogenation to methanol by a liquid-phase process with alcoholic solvents: a techno-economic analysis. *Processes*, 7(7), 405.
- Pratschner, S., Radosits, F., Ajanovic, A., & Winter, F. (2023). Techno-economic assessment of a power-togreen methanol plant. *Journal of CO2 Utilization*, 75, 102563.
- Rinaldi, R., Lombardelli, G., Gatti, M., Visconti, C. G., & Romano, M. C. (2023). Techno-economic analysis of a biogas-to-methanol process: Study of different process configurations and conditions. *Journal* of Cleaner Production, 393, 136259.
- Sollai, S., Porcu, A., Tola, V., Ferrara, F., & Pettinau, A. (2023). Renewable methanol production from green hydrogen and captured CO2: A techno-economic assessment. *Journal of CO2 Utilization*, 68, 102345.
- Sorrenti, I., Zheng, Y., Singlitico, A., & You, S. (2023). Low-carbon and cost-efficient hydrogen optimisation through a grid-connected electrolyser: The case of GreenLab skive. *Renewable and Sustainable Energy Reviews*, 171, 113033.