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To cite this article: Alessandro Ciancio et al 2023 J. Phys.: Conf. Ser. 2648 012066

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Decarbonization of methanol production - Techno-economic analysis of Power-to-Fuel process in a Hydrogen Valley

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Abstract. The European Union set the decarbonization goals and green hydrogen can play a crucial role for the greenhouse gas emission reduction. Hydrogen Valleys can be pivotal for the hydrogen economy, by integrating the local green hydrogen (H_2) production into the industrial sector. Thus, by means of the Power-to-Fuel approach H_2 can be exploited for the synthetic fuel. This study aims at investigating the synthetic methanol (CH₃OH) production process with recycled carbon dioxide (CO₂) and green hydrogen in a Hydrogen Valley. Currently, industrialscale methanol is produced from natural gas, where methane (CH_4) reacts with H_2O at high temperature and pressure. The green hydrogen can improve the long-term sustainability of this process, making the green methanol exploitable in the hard-to-abate sectors. Therefore, the purpose of this research is to evaluate a techno-economic analysis of various scenarios for the synthetic methanol production process in the Hydrogen Valley. This analysis has been carried out for different time periods: 2020, 2030, and 2050. The outcomes show that the current Levelized Cost of Methanol production ranges between 158.41 €/MWh and 227.69 €/MWh. In the long term, those values decrease to a range of 72.01 €/MWh to 97.05 €/MWh. The most suitable RES capacity scenarios have been derived along with the associated global investment costs. The best scenario in the short and medium term envisages 1 MW of on-shore wind plants and 1.5 MW of photovoltaic plants with a total investment cost of 4.10 M \in by 2020. In the long term, the best scenario foresees 2 MW of photovoltaic and 0.5 MW of on-shore wind. In so doing the 2050 investment cost is reduced to 1.62 M€.

1. Introduction

The drastic reduction of GHG emissions at global level is one of the priority objectives that must be pursued to try to mitigate the effects of climate change and not to create irreversible damage to the ecosystem and to our own health. [1]. In this context, in July 2021, with the package of legislative proposals called "Fit for 55", the European Commission raised the emission reduction targets to 55% by 2030 [2]. This transition requires a radical change in the structure and operation of the current energy system [3]. The shift to distributed energy systems is crucial for the Renewable Energy Sources (RES) integration, ensuring a great flexibility [4]. Hydrogen is a valuable element that can be easily integrated into distributed systems [5]. Green hydrogen has the potential to significantly reduce dependence on fossil fuels and help achieve global climate objectives [6]. It is produced through water electrolysis using renewable energy sources like solar or wind power.

In Italy the realization of green hydrogen's full potential faces several barriers [7]. These obstacles include high investment and operational costs, challenges in hydrogen transport and distribution, complex permit procedures, as well as safety and social concerns. Dealing with these challenges alone

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can be daunting for individual companies. Therefore, the formation of green hydrogen clusters, known as "Hydrogen Valleys," becomes pivotal in the initial stages. These Hydrogen Valleys stimulate collaboration and synergies among multiple stakeholders engaged in green hydrogen production and consumption within a specific geographical area [8].

Hydrogen Valleys are integrated ecosystems that encompass various hydrogen technologies, covering the entire value chain: from production and storage to distribution and final utilization. They represent a crucial first step towards establishing a large-scale hydrogen economy.

One of the possible end uses of green hydrogen produced in such a system could be to exploit it to produce green methanol.

Green methanol (MeOH) is one of the chemicals that can be produced from recycled CO_2 via hydrogenation technology. This product is considered a good future energy vector due to its higher volume-specific energy density and its easier transport process than other energy carriers [9]. In addition, it can also be used as a green fuel instead of gasoline in the transport sector and, in the industrial sector, as a raw material for synthetic process of many valuable chemicals (dimethylether, formaldehyde, biodiesel, etc.) [10]. Therefore, the use of green methanol can contribute to the hard-to-abate sector greening. Currently, about the 80% of the world's methanol production is done through Steam Reforming [11]. Therefore, the process of hydrogenation of CO_2 is opposed to the latter which is not a sustainable process in the long term. Nonetheless production costs are much higher for large-scale commercialization of this process. [12]

The aim of this research is to carry out a technical-economic analysis on various scenarios of green methanol production in a Power-to-Fuel process within a Hydrogen Valley inserted in a territorial context such as that of Southern Italy, in the province of Taranto.

The Power-to-X approach envisages the renewable electricity conversion into other energy carriers [13], such as a fuel like methanol. This conversion system is therefore a way to integrate the excess electricity produced by the RES, which in the future is expected to be increasingly numerous and being able to integrate their production in the most efficient way possible will be one of the technological challenges of the near future [14].

2. Methodology

2.1. Methodology Overview

The Hydrogen Valley chosen for this study is located within the territory of the province of Taranto. The production plant consists of a mix of renewable energy systems, including onshore wind and photovoltaic plants, a 1 MW size electrolyser, and a group of 4 CH₃OH reactors with a total size of 92 kg/h of methanol.

By selecting this territory as a case study, it is possible to analyse various production scenarios based on different mixes of renewables, PV, and WIND, dedicated to supplying the electrolyser. Specifically, using meteorological data on wind and solar irradiation provided by PVGis software, the hourly production profiles of PV and WIND have been derived.

Then, the hourly production profiles of various energy mixes, ranging from 0 MW to 2 MW with 500 kW steps of installed power, have been analyzed. Once the electrolyser efficiency data have been fixed, the hourly hydrogen production profile for each scenario has been obtained. Assuming that the methanol reactor is fed with the hourly hydrogen production, the annual quantity of green methanol produced was determined for each scenario using the reactor's conversion and efficiency data. These scenarios were calculated for the current condition (2020), the medium-term (2030), and the long term (2050).

Lastly, an economic analysis was carried out, by considering the installation and maintenance costs of the facilities used for local hydrogen and methanol production in each scenario. Hence, the levelized cost of the produced hydrogen and the levelized cost of methanol (LCOM) for each scenario in 2020, 2030, and 2050 has been determined. The annual CH₃OH production and the LCOM were compared to identify an optimal scenario.

2.2. Case Study

The province of Taranto has been selected for the analysis of various renewable energy scenarios for local green methanol production within a Hydrogen Valley. Twenty-two scenarios involving different WIND and PV mixes, ranging from 0 MW to 2 MW, were considered. This renewable production is used to power a 1 MW electrolyser to produce green hydrogen, which will be used, along with CO_2 recycled from anaerobic digestion processes and biomass, to fuel the methanol production system. This consists of 4 reactors, each with a size of 23 kg_{MeOH}/h. Figure 1 shows the hydrogen production scheme dedicated to supplying the methanol reactor.



Figure 1. Production scheme of green methanol in a power-to-fuel process

To obtain the hourly unit production curve for the considered renewable energy systems, the meteorological and irradiation data provided by the PVGis software have been adopted [15]. For the analysis of WIND production, wind speed data from the software was taken at specific coordinates within the territory of the province of Taranto. These coordinates were chosen based on the location of real on-shore plants currently operating in the territory, which were obtained through the Atlaimpianti portal managed by the GSE [16], to replicate the actual distribution of these plants. Through this portal, for each of these selected characteristic coordinates, it was possible to identify the actual turbines installed in those areas, allowing us to determine both the production curve of these turbines and their height. PVGis wind speed data provided at a height of 10 meters above ground level has then been converted using the logarithmic Prandtl model to make them representative of different heights above ground, considering the roughness coefficient value equal to 0.03, which is representative of open agricultural areas without fences or hedges, with widely spaced buildings, and gentle sloping hills [17]. Finally, after finding the unitary production curve for each of these characteristic coordinates, an average curve was derived to represent the territory of the province of Taranto.

To obtain the hourly production curve of PV, the PVGis software was utilized, entering the coordinates of Taranto, with an assumed tilt angle of 35° and a south orientation. The considered PV panel was made of crystalline silicon with a peak power of 1 kWp. The production curves for five years were then extrapolated and averaged to obtain a single curve for subsequent calculations.

These WIND and PV unit curves proved to be essential for analyzing various renewable energy production scenarios, which will be described below.

2.3. Energy, Production and Economic Model

To find the main parameters described above different models were used and for each of them were considered 2020, 2030 and 2050 assumptions. The energy model was implemented in MATLAB/Simulink environment for a dynamic analysis.

In order to determine the annual hydrogen production of the renewable mix scenario labeled as "k," the electrolyser total hourly energy consumption was assessed for the specific k-th scenario.

$$E_{EL_{k}}(t) = \min\{E_{W_{k}}(t) + E_{PV_{k}}(t); P_{EL}\}$$
(1)

Here:

- P_{EL} is the installed capacity of electrolyser expressed in kW. In this case, the same value is used for all scenarios. This value corresponds to the maximum hourly energy that the electrolyser can absorb in kWh.
- $E_{PV_{k}}(t)$ is the hourly energy generated in kWh by the photovoltaic plant in scenario k.

• $E_{W_k}(t)$ is the hourly energy generated in kWh by the wind plant in scenario k. The model used to calculate Prod_{H2,k} or the annual H₂ production by mass, expressed in kg_{H2}/yr, is:

$$Prod_{H2,k} = \sum_{t=1}^{8760} E_{EL,k}(t) / (LHV_{H2}/\eta_{EL})$$
(2)

In which:

- LHV_{H2} is the lower heating value of hydrogen, expressed in kWhe/kg_{H2}.
- η_{EL} is the electrolyser efficiency, expressed as a percentage.

The reaction for methanol formation or catalytic hydrogenation of CO_2 is as follows [9]:

$$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O$$
 (3)

By stoichiometric conversion factors and the reactor's efficiency value, it was possible to derive the hourly value of methanol production based on the hourly hydrogen production.

The model used to calculate the annual CH₃OH production by mass, expressed in kgM/yr, for each k scenario (Prod_{MeOH,k}) is:

$$Prod_{MeOH,k} = \sum_{t=1}^{8760} E_{EL,k}(t) / (LHV_{H2}/\eta_{EL}) \cdot fMeOH_{H2,st} \cdot \varepsilon_{MeOH}$$
(4)

In which:

- $fMeOH_{H2,r}$ is the stoichiometric quantity produced by the reaction, expressed in kilograms, for every kilogram of H₂ that reacts.
- ε_{MeOH} represents the conversion efficiency of the methanol reactor.

Lastly, the economic evaluation of the cost of hydrogen and green methanol production was conducted using the LCOH (Levelized Cost of Hydrogen) and LCOM (Levelized Cost of Methanol) parameters. These represent the ratio between the annual costs incurred from the production of hydrogen or methanol, respectively, and the amount of H_2 or CH_3OH produced annually in the given scenario 'k,' expressed in €/kg_{H2} and €/MWh_{MeOH}. It is important to note that the cost of distilled water required for the electrolysis process has been neglected in this analysis.

The cost for the required CO_2 for the methanol production has been deemed negligible [18].

$$LCOH_{k} = (C_{W,k} + C_{PV,k} + C_{EL})/Prod_{H2,k}$$

$$\tag{5}$$

$$LCOM_{k} = (C_{MeOH} + Prod_{H2,k} \cdot LCOH_{k} + Ele_{MeOH,k} \cdot C_{Ele,k})/Prod_{H2,k}$$
(6)

The economic analysis models for the annual costs related to hydrogen generation in each considered scenario k, expressed in €/yr, are as follows:

$$C_{W,k} = P_{W,k} \cdot (CAPEX_W \cdot crf_W + O\&M_W) \tag{7}$$

$$C_{PV,k} = P_{PV,k} \cdot (CAPEX_{PV} \cdot crf_{PV} + 0\&M_{PV}) \tag{8}$$

$$C_{EL} = P_{EL} \cdot (CAPEX_{EL} \cdot crf_{EL} + 0\&M_{EL}) \tag{9}$$

$$C_{MeOH} = P_{MeOH} \cdot (CAPEX_{MeOH} \cdot crf_{MeOH} + 0\&M_{MeOH})$$
(10)

Where:

- $P_{W,k}$ is the installed capacity of wind power in the considered scenario expressed in kW.
- $P_{PV,k}$ is the installed capacity of photovoltaic power in the considered scenario expressed in kW.
- P_{MeOH} is the installed capacity of methanol reactor expressed in t_{MeOH} potentially annually produced.
- $CAPEX_{W/PV/EL}$ is the capital expenditure expressed in ϵ/kW of the considered plant.
- *O*&*M*_{W/PV/EL} is the operation and maintenance cost expressed in €/kW/year of the considered plant.
- *CAPEX_{MeOH}* is the capital expenditure expressed in \notin/t_{MeOH} of the methanol reactor.
- *O*&*M*_{*MeOH*} is the operation and maintenance cost expressed in €/t_{MeOH}/year of the methanol reactor.
- *Ele_{MeOH,k}* is the annual electricity consumption for methanol reactor in the considered scenario expressed in MWh/t_{MeOH}.
- C_{Ele} is the electricity cost expressed in \notin /MWh.
- $crf_{W/PV/EL/MeOH}$ is the capital recovery factor which can be computed as follows:

$$crf_{W/PV/EL/MeOH} = \frac{i \cdot (1+i)^{\tau_{W/PV/EL/MeOH}}}{((1+i)^{\tau_{W/PV/EL/MeOH}}-1)}$$
(11)

Here, *i* represents the interest rate of investments and τ is the lifetime. Calculate it for both wind turbines, PV, electrolyser, and methanol reactor.

2.4. Technical and Economic Assumptions

The main assumptions made for the development of the energy and production model regards both the electrolyser model and the choice of methanol reactor.

For the electrolyser, the following parameters was considered:

- Typology PEM,
- Size $P_{EL}=1$ MW,
- LHV efficiency, equal to 64% for 2020, 69% for 2030 and 74% for 2050 [18][[19]
- Output H₂ flow rate equal to 200 m3/h [19]

For the green methanol production, the catalytic hydrogenation reaction of CO₂ was considered, using an adiabatic fixed-bed catalytic reactor operating at a working pressure of 80 bar, temperature of 240 °C, with a molar H₂-CO₂ ratio of 3:1, and a conversion efficiency of 96% [20]. These are typical process values when using Cu/Zn/Al-based catalysts [9]. To determine the reactor size, it was scaled based on the nominal output hydrogen flow rate from the electrolyser. Using this value, a size of 92 kg_{MeOH}/h was defined. However, as partial operation of the electrolyser was also considered, the hydrogen output will not always match the nominal value. Therefore, it was decided to split the 92 kg_{MeOH}/h into four reactors of 23 kg_{MeOH}/h each. This decision was made due to the high inertia of chemical reactors; therefore, the methanol synthesis plant should operate at a maximum of 75% of nominal conditions. The assumptions underlying the economic model used are reported in Table 1.

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	Unità di misure	2020	2030	2050	Source
CAPEXw	€/kW	1,473	1,075	825	[21], [22]
CAPEX _{PV}	€/kW	995	587	325	[21], [23]
CAPEX _{EL}	€/kW	900	700	450	[18]
CAPEX _{MeOH}	€/t _{MeOH}	322	242	155	[18], [24]
O&Mw	€/kW/yr	30.00	21.50	16.50	[18], [21], [22]
O&M _{PV}	€/kW/yr	10.00	5.87	3.23	[21], [23]
O&Mel	€/kW/yr	13.50	10.50	6.75	[18]
О&Ммеон	€/t _{MeOH} /yr	4.82	3.63	2.32	[18]
Еlемеон	MWh/t_{MeOH}	0.43	0.40	0.38	[18], [24]
CEle	€/MWh	199	231	250	[18], [25]

T	4	- ·		
Table	1.	Economic	assum	ptions

During PEM electrolysers lifetime, the replacement of the stack, primarily consisting of bipolar plates and the membrane. These replacement interventions are encompassed in the considered CAPEX costs and constitute a significant percentage of the investment cost:

- Stack Lifetime: 10 yr.
- Stack Replacement Cost: 40% of capital cost [26].

Finally, the interest rate of investment was assumed equal to 3%, while other assumptions on lifetime are reported in Table 2.

	Lifetime of the plant, τ [yr]	Source
WIND Plant	25	[22]
PV Plant	25	[23]
Electolyser	20	[18]
Methanol Reactor	25	[18]

Table	2.	TLT	of	princi	pal	plant
			~ -	P	P ***	

3. Results and Discussion

To produce green methanol within the province of Taranto, it will be necessary to plan the installation of a specific renewable energy mix to supply the electrolysers for green H_2 production, which will then be fed into the reactor along with recycled CO₂. For the assumed conditions, the emissions factor for this CO₂ is considered negligible.

A total of twenty-two scenarios involving various combinations of WIND and PV systems ranging from 0 to 2 MW were analysed to determine:

- The annual hydrogen production using a 1 MW electrolyser.
- The methanol production using a group of reactors with a total nominal size of 92 kg_{MeOH}/h.
- The LCOH (Levelized Cost of Hydrogen)
- The LCOM (Levelized Cost of Methanol)

All these parameters were evaluated for each scenario in the short, medium, and long term. In Figure 2-Figure 5 the 2020 results of these parameters for each scenario are presented.

2648 (2023) 012066 doi:10.1088/1742-6596/2648/1/012066



Figure 2. Trend of the annual hydrogen production value as a function of the installed PV and WIND capacity for 2020



Figure 3. Trend of the annual MeOH production value as a function of the installed PV and WIND capacity for 2020



Figure 4. LCOH value trend as a function of the installed PV and WIND capacity for 2020

2648 (2023) 012066 doi:10.1088/1742-6596/2648/1/012066



Figure 5. LCOM value trend as a function of the installed PV and WIND capacity for 2020

It can be observed that both H_2 and MeOH production increase with the installation of higher renewable power capacities. In the medium and long term, thanks to the predicted increase in the efficiency of the electrolysers, the range will vary from 30.3 to 118.5 t_{H2}/yr and from 155.4 to 606.8 t_{MeOH}/yr in 2050. From Figure 4Figure 5 it is noticeable that LCOH and LCOM are higher in scenarios with fewer installed renewables. This is because in these scenarios, the production of H_2 , and consequently CH₃OH, will be significantly lower, impacting the production cost more than the cost of larger-scale facilities. In the short term, the market price of conventionally produced methanol has a production cost of about 80 ϵ /MWh, which is much lower than the resulting LCOM from the analysed scenarios. In the medium and long term, due to the expected decrease in investment costs of renewable systems and electrolysers, as well as an increase in PEM production efficiency, the value of LCOH will significantly decrease, leading to a reduction in LCOM alongside a decrease in reactor costs.

Indeed, by 2050, it is projected that the range for LCOH will be from 1.41 to $2.10 \notin kg_{H2}$, and for LCOM, it will vary from 72 to 97 \notin /MWh.

The cost values mentioned above could potentially make the green methanol production system (powerto-fuel) competitive with the conventional ones produced from fossil sources in the future. To identify the optimal production scenarios, the obtained results have been graphed based on the LCOM value and the annual methanol production for 2020, 2030, and 2050, as shown in Figure 6-Figure 8.





2648 (2023) 012066 doi:10.1088/1742-6596/2648/1/012066





Figure 8. Comparison between the annual methanol production value and the LCOM value for each of the considered scenarios in 2050

From Figures 6-8, it is possible to identify a Pareto front that helped to determine the best compromise between the two outputs. The optimal scenario for 2020 and 2030, regarding the power-to-fuel system, consists of 1.5 MW of PV and 1 MW of WIND. For both considered periods, this scenario proves to have the lowest cost value while maintaining good production values compared to others. For 2050, however, the optimal scenario is composed of 2 MW of PV and 0.5 MW of WIND. This has the second lowest LCOM value but a considerably higher annual production value than the first. Compared to 2020 and 2030 best scenario, the percentage of photovoltaic capacity will be higher. This can be attributed to a more rapid decrease in photovoltaic costs expected in the long term compared to that of WIND installations.

4. Conclusion

This study aims to propose an analysis to identify short, medium, and long-term optimal scenarios for renewable energy power plants dedicated to a power-to-fuel plant for green methanol production within a Hydrogen Valley in the territory of the province of Taranto. The study seeks to highlight the green hydrogen deployment for the hard-to-abate sectors greening, by supporting the energy transition towards carbon neutrality. The produced green methanol can be used as an electrically derived fuel (e-fuel)

directly in the transport sector as an alternative to traditional fuels - Road transport stands out as one of the most polluting sectors due to its heavy reliance on fossil fuels, surpassing that of any other industrial sector [27] - or as a building block for numerous chemical processes that currently rely on fossil fuel-derived methanol.

From the analysis of all the various scenarios considered, it was found that in the short term, the ideal scenario is the one composed of 1 MW of WIND and 1.5 MW of PV that allows the production of 387 t_{MeOH}/yr with a levelized cost of 158.40 ϵ /MWh and an initial investment of 4.10 M ϵ . For the medium term, the ideal scenario remains the same; however, the investment and production costs decrease to 2.83 M ϵ and 109.03 ϵ /MWh, respectively, while the production increases to 418 t_{MeOH}/yr . In the long term, the ideal scenario will be the one composed of 2 MW of PV and 0.5 MW of WIND which leads to an annual production of 393 t_{MeOH}/yr with investment and LCOM costs of 1.62 M ϵ and 72.57 ϵ /MWh, respectively. The production cost of green methanol is still not competitive with conventionally produced methanol from fossil sources, but by 2030 and 2050, this gap is expected to be closed. The results obtained align with the IEA's predictions, which estimate the cost range of green methanol in the short term to be between 125 and 210 ϵ /MWh and in the long term between 60 and 80 ϵ /MWh [28].

It is essential to note that the cost of conventional methanol does not account for external costs related to CO_2 emissions and other environmental and health impacts. Therefore, its production based on fossil sources is not sustainable in the long term. The future trends envisage centralized RES. Hence, increasing renewable energy production is foreseen along with lower investment and production costs.

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