TECHNO-ECONOMIC ANALYSIS OF RENEWABLE METHANOL PRODUCTION AT GIGAWATT SCALE – UTILIZING GREEN HYDROGEN FOR DIRECT CO2 HYDROGENATION

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ABSTRACT

As part of the European project Hy2Market, the use of green hydrogen in refineries will be investigated. One possible use case of green hydrogen is the production of renewable methanol by means of direct CO_2 hydrogenation, which will be examined in this paper. In the course of this work, a techno-economic analysis of renewable methanol production at gigawatt scale was carried out. Such scales have an impact on a country's infrastructure and have not been realized yet. Throughout this study efficiencies and energy balances of a base case scenario are investigated and visualized in a sankey diagram. Renewable electricity is produced either with wind, solar or a combination of it. The dynamics of the electrolyzer are taken into account to reflect the fluctuation of renewables. At this scale, large storage quantities are necessary. The aim of this work is to examine the required storage capacities for hydrogen including large scale storages (underground) as well as intermediate and short-term storages (pressure, liquid, metal hydrides, liquid organic hydrogen carrier) to identify the most suitable solution for renewable methanol production. The system simulations were done in Modelica/Dymola, which enables a dynamic view of the system. Furthermore, the conducted techno-economic analysis shows that renewable methanol can be produced for less than 1000 €/t.

1 INTRODUCTION

Hydrogen based e-fuels can be seen as alternative source where electrification is challenging, like aviation and the chemical industry. (Campion *et al.,* 2022). Methanol is playing a key role in the chemical industry, as it is used as feedstock for many chemicals, such as polyolefins produced through a subsequent methanol to olefin (MTO) process. Another important area of application for methanol is the production of sustainable aviation fuel (SAF) to decarbonize the aircraft sector (IRENA and METHANOL INSTITUTE, 2021). With the ReFuelEU initiative, the EU will set binding quotas for SAFs for all airlines in future, with 6% of aircraft fuel being replaced by SAFs by 2030 (EU PARLIAMENT & COUNCIL, 2023). Nearly all of today's methanol is produced from fossil fuels. CO_2 emissions from existing methanol production account for 10% of the whole chemical sector. Renewable methanol has the potential to substitute fossil-based hydrocarbons, as it can be produced entirely from renewable sources like photovoltaics (PV) and wind. Current methanol production was about 98 Mt/ year in 2019 and is expected to rise to 120 Mt by 2025 and 500 Mt by 2050, which would release 1.5 Gt CO_2 per year if its entirely sourced from fossil fuels. The production of renewable methanol is currently less than 0.2 Mt per year, mainly due to higher production cost compared to methanol derived from fossil sources. Main cost drivers are feedstock (H_2 and CO_2) and plant costs. (IRENA and METHANOL INSTITUTE, 2021) Depending on CO_2 source IRENA and the Methanol Institute stated in their report of 2021 current renewable methanol costs between 800 and 2400 USD/t. However renewable electricity is expected to decrease over the next decades, and it can also be assumed that electrolyzers will become cheaper because of innovation and economy of scale. According to IRENA and the Methanol Institute costs will decrease to levels of 250 to 630 USD/t by 2050.

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2 Renewable Methanol Synthesis

In principle renewable methanol is produced with renewable energy and renewable feedstocks. Based on the source of the feedstock a distinction between bio-methanol and green e-methanol is made. Bio-methanol is based on sustainable biomass as a feedstock, whereas green e-methanol uses captured CO_2 from bioenergy or directly from the air and green hydrogen derived from electrolysis powered by renewable electricity. Renewable methanol via both routes is chemically the same as produced from fossil sources. Due to its properties (liquid at ambient pressures and temperatures) it is easy to store and distribute with an existing infrastructure. (IRENA and METHANOL INSTITUTE, 2021)

2.1 Process

As it can be seen in **Figure 1**, the system for renewable methanol production consists of an available CO_2 source derived from a capturing unit or the grid, hydrogen production through electrolysis, hydrogen storage and the actual methanol synthesis step. The electricity for electrolysis is obtained from various sources, like wind, PV, hydro power, or the electrical grid. Methanol is produced throughout direct CO_2 hydrogenation. A subsequent further processing step of methanol is not considered in the course of this work.

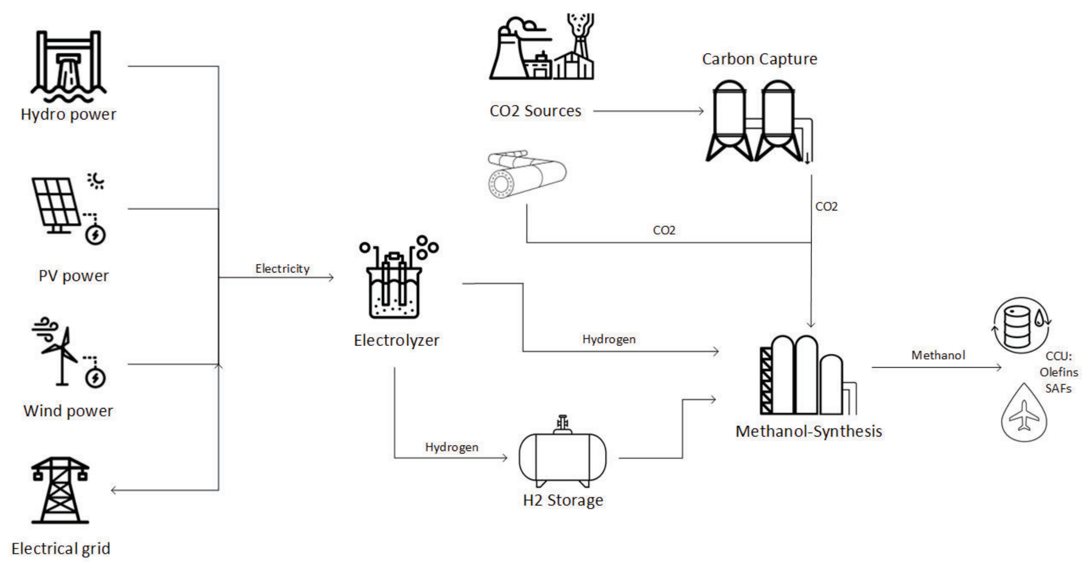

Figure 1: System for renewable methanol production.

The examined methanol synthesis is a typical low-pressure process with a recycle loop due to its chemical equilibrium limitation. This means the reactor outlet consists of products and unreacted educts, which are separated after cooling down. The condensed products are then separated in a distillation column. (Kiss *et al*., 2015) Methanol reactors are operated at 200-300°C and 50-100 bar and have a stoichiometric number of two at the reactor inlet. (Rahimpour *et al*., 2023)

2.2 Use Case

The investigated scenario is a full-scale renewable methanol production in the eastern region of Austria. To meet a major part of future demand for olefins and sustainable aviation fuels (SAF) based on methanol, the scenario in this use case assumes that approximately 1.3 million tons of renewable methanol per year will be produced.

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3 Modelling

For this purpose, a dynamic model of the renewable methanol production, as shown in Figure 1, was developed in Modelica/Dymola. The comprehensive simulation framework facilitates a holistic assessment of renewable methanol production to provide insights into the feasibility and efficiency of the process. The dynamic modeling allows to account for the fluctuating energy production and its effects on the system. **Figure 2** shows the modeled system including renewable electricity production (wind and pv) with actual weather data (upper left of **Figure 2**). The electricity of wind and pv is summed up and depending on the dynamics of the electrolyzer limited before it will be fed into the electrolyzer, which will then produce hydrogen. This hydrogen is either stored in a model component based on pressure and volume or fed into the methanol synthesis. The CO_2 source is considered to be available and is fed into the synthesis loop according to the stoichiometric ratio. This means for the purpose of this paper capturing CO_2, storage and transport were not taken into account.

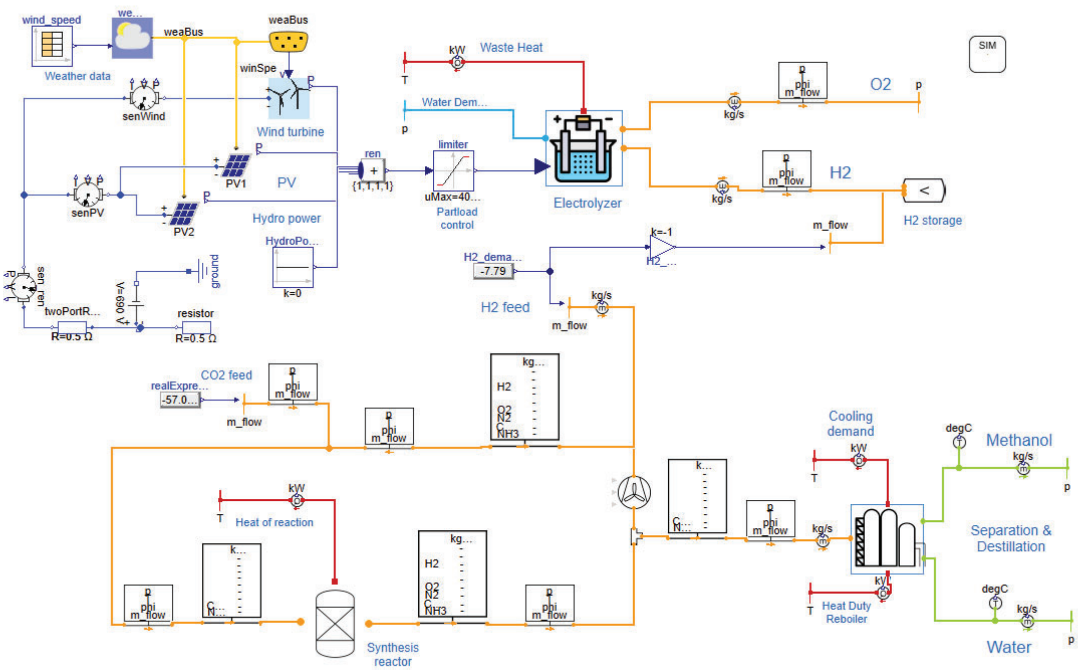

Figure 2: Dymola model of renewable methanol production.

H_2 and CO_2 mixture is fed into the reactor and is converted into methanol and water based on stoichiometry and conversion rates (lower left of **Figure 2**). The produced mixture is then split up into its pure components in a simple distillation component with specific energy demands as input parameters (lower right of **Figure 2**). The system consists of grey-box models of the individual components, which are based on physical characteristic curves. The most important components in the system are briefly described below.

3.1 Renewable electricity production

Based on actual weather data from EnergyPlus and New European Wind Atlas renewable energy production is calculated. Especially geographically sensitive wind data was validated with data from manufacturers. Wind power is calculated with a turbine specific power curve, which can be seen in **Figure *3***. Wind speed data is generally at a height of 10m. To account for different heights of turbines, windspeed at a specific height is calculated with a correction factor.

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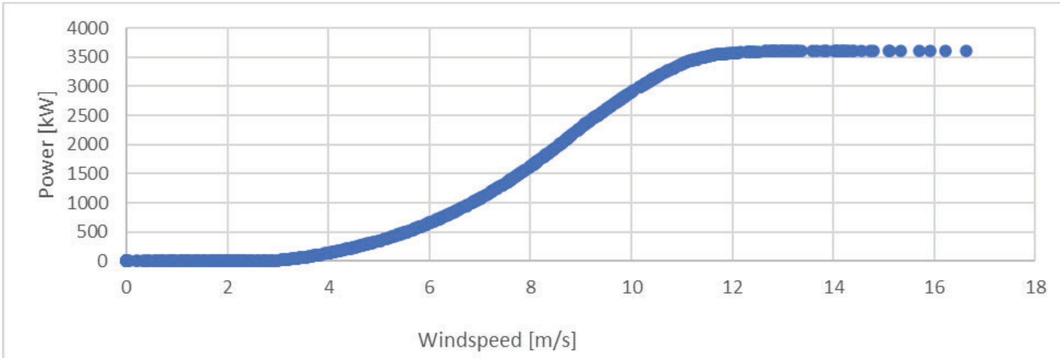

Figure 3: Power curve of wind turbine Enercon E-101 E2 with a nominal power of 3.6MW.

The plot shows the power curve of the turbine type which is used in the model. It has a height of 74m above ground and a cut-in/ cut-out wind speed of 2.5 m/s and 25 m/s respectively. (Bauer and Matysik, 2024). PV power is calculated with total irradiation from weather data, which consists of diffusive and direct irradiation. Generated power by means of photovoltaics is calculated based on following equation:

$$P = G * A * \eta * f(\varphi, \theta) \tag{1}$$

where:

G…Total irradiance [W/m²]
A… Effective surface area of modules [m²]
η… Efficiency [-]
φ… Surface tilt [°]
θ… Surface azimuth [°]

Hydropower can be implemented in the model as a variable power profile but is not relevant for the use case under consideration due to the geographical location.

3.2 Electrolysis

Hydrogen production throughout electrolysis is modeled as grey-box model based on the polarization curve (U-i characteristic) of an electrolyzer, which relates to the different losses in an electrolytic cell, namely activation-, mass transfer-, and ohmic losses. Siemens published a whitepaper with characteristic curves of Polymer electrolyte membrane (PEM) and alkaline electrolysis (AEL), which are shown in **Figure 4** and implemented in the model. (Siemens Energy, 2020)

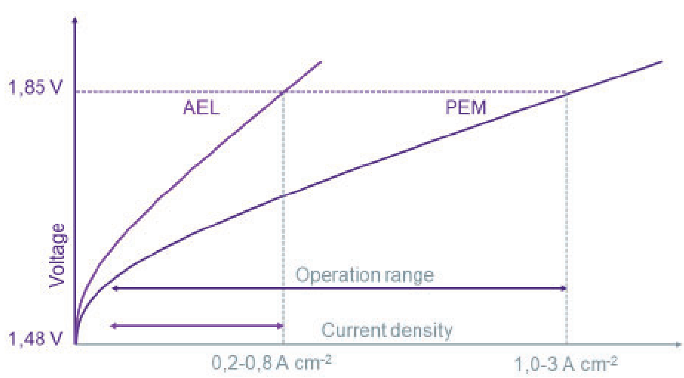

Figure 4: Characteristic U-i curve of PEM and AEL. (Siemens Energy, 2020)

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The curve shows the actual cell voltage of an electrolyzer cell with the associated current density. This means that the electrolyzer has a higher efficiency in part-load. The operational range of AEL is significantly lower than PEM. The produced hydrogen is directly correlated to the current in the electrolyzer, as stated in Equation (2).

$$\dot{n}_{H2} = \frac{I}{z*F} \tag{2}$$

where:

$\dot{n}_{H2}$... Molar flow of hydrogen [mol/s]
I... Current [A]
z... Number of mole of electrons per mole of hydrogen participating in the reaction [-]
F... Faraday constant [C/mol electrons]

Reversible and thermoneutral voltage of the cells is assumed to be constant and have the values 1.23V and 1.43V respectively.

3.3 Methanol synthesis

For the system simulation methanol synthesis is modeled as grey-box with an recycle loop, because of the equilibrium limitation of the process. The feed streams H_2 and CO_2 are fed in these recycle loop. Mass balance is calculated according to the stoichiometry of following chemical reactions: (Kiss *et al*., 2015)

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

$$CO + 2H_2 \rightleftharpoons CH_3OH$$

with a reaction enthalpy of -49.2 kJ/mol for CO_2 hydrogenation and -90.8 kJ/mol for CO hydrogenation. Heat of reaction is calculated based on the reaction enthalpy. Conversion rates (X_{CO2} & X_{CO}) are derived from input and output streams and are given as parameters. Produced species are calculated based on conversion rates and stoichiometry, seen in Equations (3) and (4). (Kiss *et al*., 2015)

$$\dot{n}_{H2O,out} = \dot{n}_{H2O,in} + X_{CO2} * \dot{n}_{CO2,in} \tag{3}$$

$$\dot{n}_{CH3OH,out} = \dot{n}_{CH3OH,in} + (X_{CO2} * \dot{n}_{CO2,in} + X_{CO} * \dot{n}_{CO,in}) \tag{4}$$

The separation and distillation stage are also modeled as grey- box with specific heat demand and duty based on manufacturer information. The water/methanol mixture is split according to the mass balance. The overall additional heat demand for distillation is calculated as follows (Kiss *et al*., 2015),

$$\dot{Q}_{MeOH\ synthesis} = \dot{Q}_{Reboiler} - \dot{Q}_{Reaction} \tag{5}$$

This means in the base case scenario it is assumed that the reaction heat in the methanol reactor is used for the reboiler duty in the distillation column.

4 Simulation results

In the following section the result of a base scenario of the use case will be presented as well as some specific selected scenarios. Simulations are carried out for a whole year of production with a resolution of 1 minute. The base case scenario is a constant methanol production of roughly 1200 kilo tons per year including a large-scale hydrogen storage.

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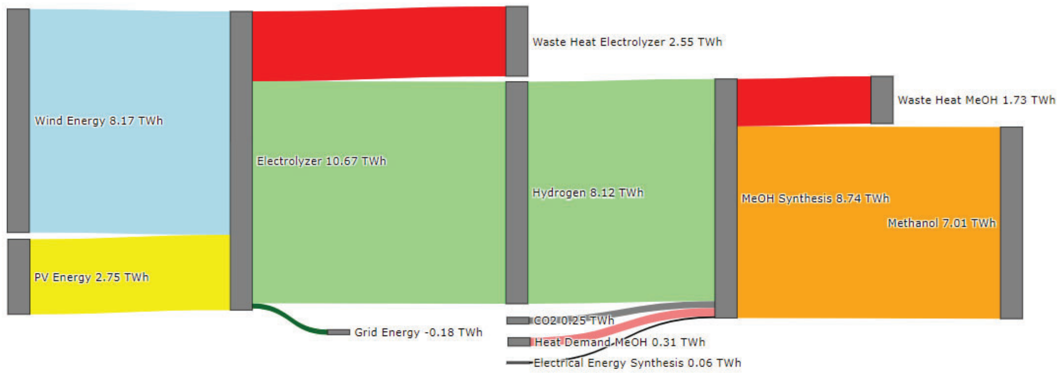

Figure 5: Sankey diagram of base case scenario.

The energy balance of one year for the different components in the renewable methanol system can be seen in **Figure 5**. The efficiency of the overall process is approximately 65%. In this system a waste heat recovery from the exothermic reaction to the reboiler of the distillation column is considered. The remaining waste heat of methanol synthesis is due to cooling demands in the distillation column.

4.1 Renewables and electrolyzer

Based on total irradiation and windspeed of eastern Austria, generated electricity within PV and wind turbines is calculated. For the base scenario the total installed renewable power is 4.6 GW peak, which is split to 2.4 GW wind power and 2.2 GW PV power. In contrast to PV systems, wind power systems have no significant summer/winter fluctuation but are nevertheless highly dynamic. This results in a weakened seasonality of the total produced renewable electricity, as it can be seen in **Figure 6**. The capacity factor wind and PV is 0.38 and 0.14 respectively, which are on the upper bounds but in the usual range.

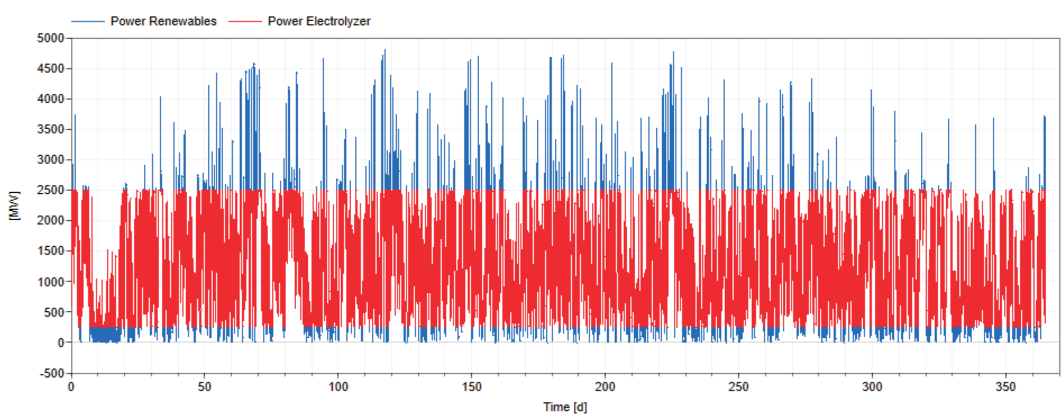

Figure 6: Renewable energy production and electrolyzer power.

Electrolyzers in the model can be operated in part load as a percentage of the nominal power and can handle all power ramps. For the base case scenario, the nominal load is 2.5 GW and the minimum part load for the PEM electrolyzer is 10%, which can be seen as the upper and lower boundaries of the red curve in **Figure 6**. If renewable energy production is below that threshold, power from the grid is used. Surplus electricity above the nominal power of the electrolyzer is fed into the grid. The capacity factor of the electrolyzer is 0.49. Based on the power input and the characteristic U-i curve of the electrolyzer, a variable efficiency results. Generally, an electrolyzer cell has higher efficiencies in part load, which

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can be seen in **Figure 7**. Efficiency for PEM is in between 70-77%, which is in the usual range of new electrolyzers.

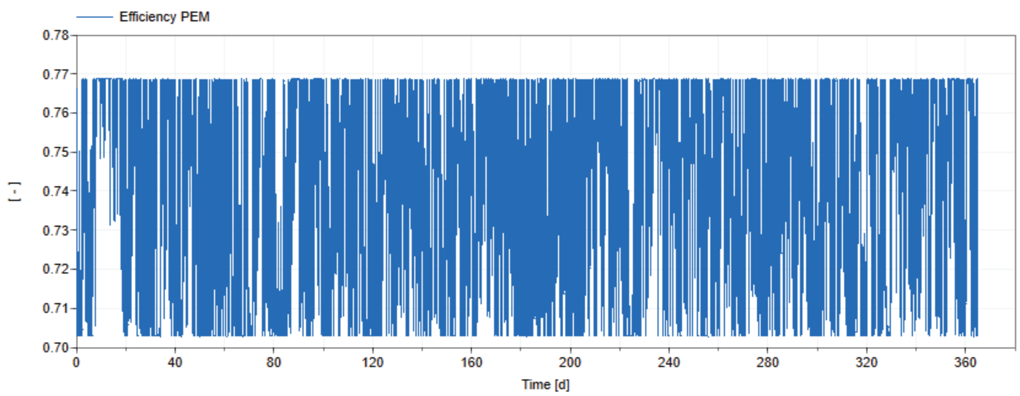

Figure 7: Variable efficiency of PEM electrolysis based on U-i characteristic.

As the produced hydrogen is directly related to the current, which is derived from the power input into the cell, a dynamic hydrogen production correlated to renewable electricity results and can be seen in **Figure 8**. As the electrolyzer has a maximum power of 2.5 GW, hydrogen production is capped at approximately 15 kg/s. In the base case scenario, a constant methanol production is assumed. This means that also hydrogen demand for methanol synthesis is constant, which can be seen by the red line in **Figure 8**. This diagram is also the basis for the following storage considerations in the paper.

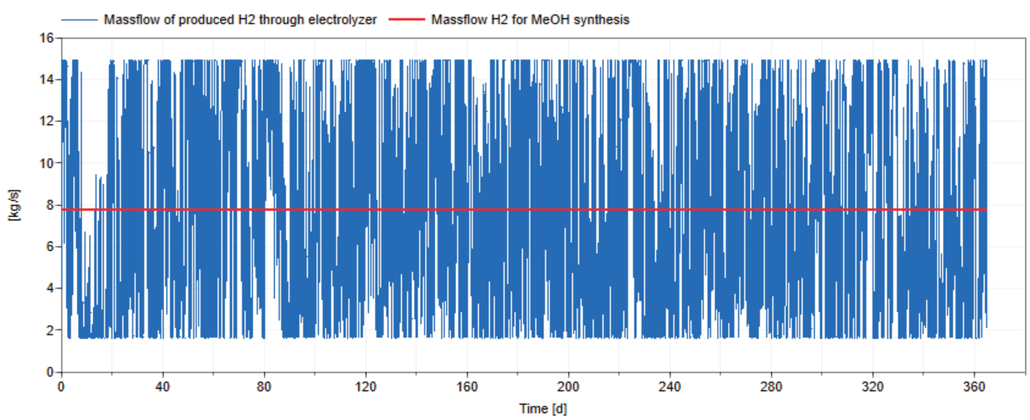

Figure 8: Produced hydrogen based on actual current in the electrolyzer.

H_2 production over one year shows a significant period without renewable energy production in January, which must be bridged using a hydrogen storage. In order to assess the seasonality of electricity and hydrogen production, the respective time series from **Figure 6** and **Figure 8** were accumulated on a monthly basis and are shown in **Figure 9**.

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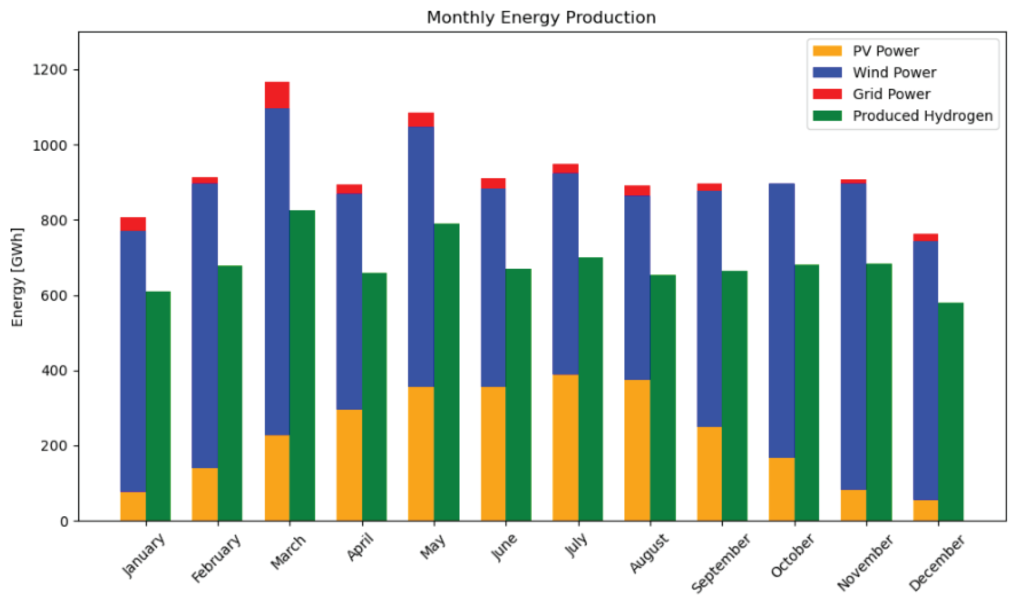

Figure 9: Monthly renewable energy and hydrogen production.

It can be seen, that in the summer months electricity production from wind is lower than the rest of the year. This mean electricity generation from wind and PV complement each other very well at the location of the base case scenario in eastern Austria. For this reason, the seasonal fluctuations in hydrogen production for this scale is reasonable. Nevertheless, there are storage demands on a smaller timeframe, due to the dynamic fluctuations of wind and PV. The next section will focus on the hydrogen storage requirements in more detail.

4.2 Hydrogen storage

Assuming a constant methanol production with dynamic electricity production according to renewables results in a hydrogen storage demand curve. **Figure 10** shows the filling level of a hydrogen storage over a whole year. Although monthly hydrogen production is relatively constant, there is a slight seasonality in hydrogen production.

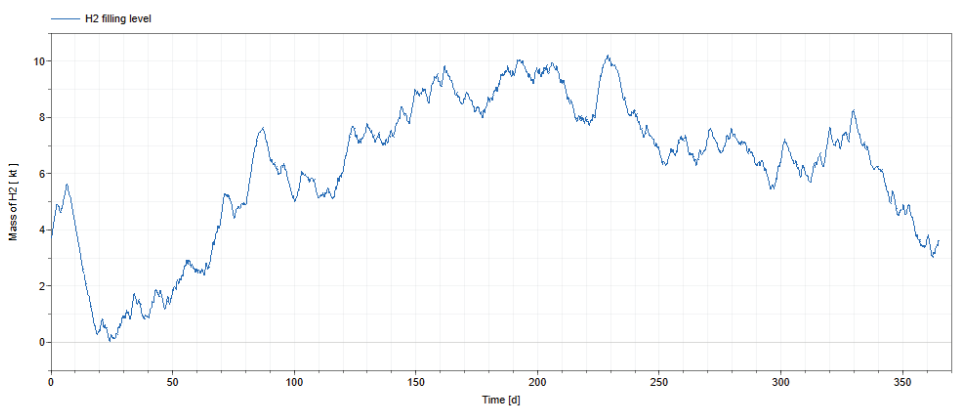

Figure 10: Hydrogen filling level in storage over one year.

It is also noticeable that there are significant peaks in shorter periods of time. To illustrate this a shorter timeframe was plotted in **Figure 11** and compared with the highly dynamic hydrogen production throughout the electrolyzer.

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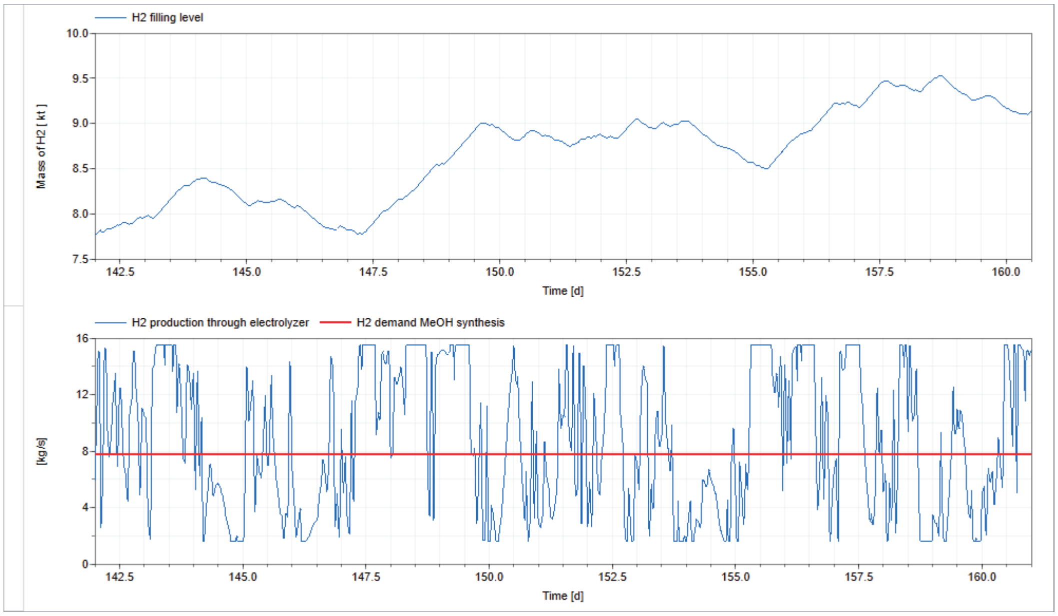

Figure 11: Hydrogen production and demand (below) and corresponding storage filling level (above).

This means storage considerations must be carried out over a wide range of time periods. The simulations give the necessary mass storage quantities of pure hydrogen. In the following different storage technologies were compared based on mass and volume of the storage. For this reason, the following volumetric densities and the potential hydrogen content from Usman (2022) in **Table 1** were considered.

Table 1: Density and storable mass of different H_2 storage types. (Usman, 2022)

Type of storage	Volumetric density [kg/m³]	H_2 content [wt% H_2]
Pressurized vessel (350bar) without tank	24.5	100
Pressurized vessel (700bar) with tank	40.8	5.7
Liquid hydrogen (-253°C) with tank	51	14
Metal Hydride (MgH2)	110	7.5
Metal Hydride (FeTiH2)	114	1.89
LOHC (Benzyltoluene)	50	6.2

From the storage demand curve in **Figure 10**, the required mass of hydrogen that needs to be stored was extracted for different time frames, especially in times of low hydrogen production. In **Table 2** the corresponding storage volume of different technologies were calculated.

Table 2: Volume of different H_2 storage types.

Type of storage	Unit	Year	Month	Week	Day
Mass of hydrogen	kt	10.2	4.42	3.27	0.52
Underground storage (350bar)	m³	416'327	180'408	133'469	21'224
Pressurized vessel (700bar)	m³	250'000	108'333	80'147	12'745
Liquid hydrogen (-253°C)	m³	200'000	86'667	64'118	10'196
Metal Hydride (MgH_2)	m³	92'727	40'182	29'727	4'727
Metal Hydride ($FeTiH_2$)	m³	89'474	38'772	28'684	4'561
LOHC (Benzyltoluene)	m³	204'000	88'400	65'400	10'400

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Due to the already mentioned period of approximately 2 weeks in January with very small H_2 production due to less wind and sun, the storage requirements on a monthly and weekly basis are similar. To make these numbers more tangible, a weekly storage system based on metal hydrides would require approximately 900 standard 20-feet ship containers. The table below shows the required mass based on the storable mass in weight percent.

Table 3: Mass of different H_2 storage types.

Type of storage	Unit	Year	Month	Week	Day
Mass of hydrogen	kt	10.2	4.42	3.27	0.52
Underground storage (350bar)	kt	10.2	4.42	3.27	0.52
Pressurized vessel (700bar)	kt	178.95	77.5	57.4	9.123
Liquid hydrogen (-253°C)	kt	72.86	31.6	23.4	3.7
Metal Hydride (MgH_2)	kt	134.2	58.2	43	6.8
Metal Hydride ($FeTiH_2$)	kt	539.7	233.9	173	27.5
LOHC (Benzyltoluene)	kt	164.5	71.3	52.7	8.4

It can be seen that H_2 storage capacities at gigawatt scale are getting very large. Therefore, storage considerations must include different technologies and different time scales or a combination of it.

4.3 Costs

In this section levelized cost of methanol will be calculated according to the presented results above. A total amount of 1267 kt of methanol is produced per year, which requires 243 kt of H_2 and 1790 kt of CO_2. Levelized costs contain CAPEX and OPEX of the different components (renewables, electrolyzer, H_2 storage and methanol synthesis including distillation, based on the cost assumptions in **Table 4**. Installed power of PV and wind are 2.2 GW and 2.4 GW respectively. Size of compressor is assumed to be 2 t/h with a specific electricity demand of 2.2 kWh/kg. (Talukdar *et al.,* 2024) For the base case scenario, the maximum mass flow to the hydrogen storage is 27.7 t/h, this results in 14 compressors which are needed for the system. Total length of wells to be retrofitted is assumed to be 5km.

Table 4: Cost Assumptions CAPEX and OPEX of different technologies. Costs of hydrogen storage based on Talukdar *et al.* (2024).

Specific costs	Unit	CAPEX	OPEX
Wind	€/kW	1000	30
PV	€/kW	610	10
Electrolyzer	€/kW	1000	50
Methanol synthesis	€/t	200	10
H_2 Compressor (storage)	€/#	9.5 Mio	*
Wells (retrofit)	€/km	270,000	-

*) Calculated with specific electricity demand of compressors, massflow of hydrogen to storage and electricity price of the grid.

Additionally to CAPEX financing cost are calculated with compound interest rates with Equation 6 and the assumptions in **Table 5**.

$$K_n = K_0 * \left(1 + \frac{i}{100}\right)^n \qquad (6)$$

Costs for the electricity grid were calculated by offsetting feed-in and feed-out with the same price. Heat demand for the system was calculated according to Equation 5. The price of electricity and CO_2 is an estimate based on discussions with industrial partners for the future price of carbon dioxide derived from biogenic sources.

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Table 5: Economic parameters and cost assumptions.

Economic parameters / prices	Unit	Value
Lifetime of assets	a	20
Interest	%	5
Electricity price (grid)	€/MWh	80
CO_2	€/t	150
Process heat	€/MWh	16

One year was simulated and the produced quantities were extrapolated to the lifespan of the system. The levelized cost of methanol can be seen as the sum of levelized costs of all components in the system. Referenced to the renewable energy production levelized cost of wind are roughly 40 €/MWh and for PV 65 €/MWh, what results in total levelized cost of renewables of 46 €/MWh. Adding the electrolyzer cost to renewables and referenced to the total amount of hydrogen produced results in levelized cost of hydrogen of roughly 3.4 €/t. Levelized cost of methanol are calculated by total costs of all components and standardized to the total amount of renewable methanol produced, as it can be seen in **Figure *12***. Levelized cost of the base scenario is roughly 920 €/t.

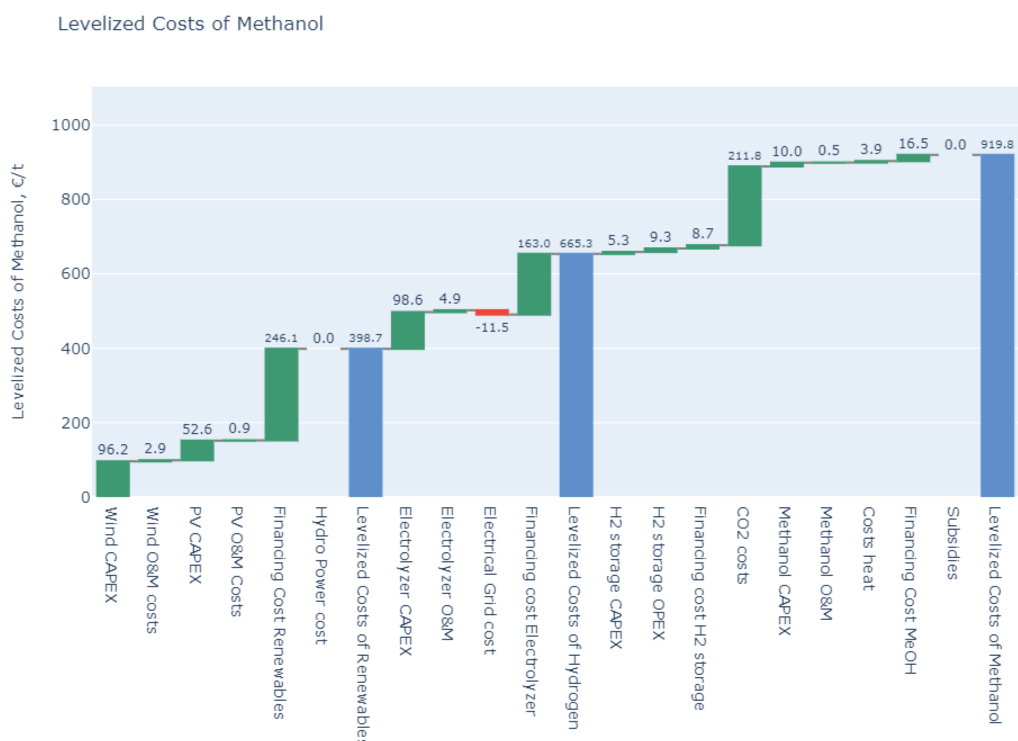

Figure 12: Levelized cost of renewable methanol for base case scenario.

Financing cost are a major part of total levelized cost of methanol. At interest rate of 5% per annum and a lifetime of 20 years, it accounts for roughly 50% of the costs. Other main cost drivers are CAPEX of renewables and electrolyzer, as well as CO_2 costs. Costs for hydrogen underground storage and CAPEX of methanol synthesis play a minor role regarding total costs. Negative grid costs, as it is indicated by the red bar in **Figure 12**, arises from the design of the renewable and electrolyser system, as in **Figure 6**, which results in a net feed into the grid. Switching electrolyzer to AEL technology results in lower CAPEX, but at the same time the required renewable energy systems are increasing due to lower efficiency of the AEL. This almost balances out the total levelized cost of methanol.

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5 Conclusion and Outlook

Renewable methanol can be a viable precursor for chemicals and SAFs, as it can be produced fully renewable. Results have shown that methanol can be produced with an efficiency slightly above 60% assuming a waste heat utilization from the methanol synthesis reactor. Renewable energy production in eastern Austria demonstrate that PV and wind complement each other well, what results in less seasonal storage demand. Although storage demands on a smaller timescale are quite high with 4.4 kt on a monthly and 3.3 kt on a weekly basis. As Sollai *et al.* (2023) also stated that main cost drivers for renewable methanol are CAPEX for renewables and electrolyzers, financing costs and CO_2 as a feedstock, same conclusion is drawn based on this study. On the other hand, seasonal hydrogen underground storage plays a negligible role. In summary, the results show that with a system at gigawatt scale using both AEL and PEM electrolyzers it is possible to produce methanol under 1000 €/t.

NOMENCLATURE

MTO	Methanol-to-Olefins
SAF	Sustainable aviation fuel
PEM	Polymer electrolyte membrane
AEL	Alkaline electrolysis
LOHC	Liquid organic hydrogen carrier

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