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Abstract:

Sectors such as aviation, shipping, and the chemical industry face challenges to abate their greenhouse gases emissions (GHGs) due to the technical limits of direct electrification. One option often mentioned to reduce the climate impact of these sectors is the use of e-fuels produced from electrolytic hydrogen and nitrogen or carbon. E-fuels are usually called green fuels assuming that 100% of the electricity used to produce the hydrogen originates from renewable power and that carbon is biogenic. However, a local plant optimization suggests that using backup power from the grid limits storage investments, plant oversizing, and, for a given fuel demand, significantly diminishes the e-fuel production cost compared to an off-grid renewable system. This paper presents a method to estimate the life cycle GHGs emissions of e-fuels produced from local renewable power and grid electricity while minimizing production costs. Focusing on e-ammonia, we found that with 2019 hourly grid emissions and prices, the least-cost solution in North Chile (with large solar potential) uses 58% of grid electricity and emits 183 $gCO2_e/MJ_{NH3}$. In Denmark, the cheapest option uses 100% of electricity from the grid and emits 109 $gCO2_e/MJ_{NH3}$. Compared with the 136 $gCO2_e/MJ_{NH3}$ life cycle emissions of ammonia produced from natural gas, this result shows the importance of green grid electricity and transparent emissions tracking and accounting, or a restrictive usage of grid power to avoid the production of "cheaper but dirtier" e-fuels.

Keywords:

Hydrogen; Carbon footprint; Ammonia; Methanol; Optimization; Emissions; Sustainability

1. Introduction

Hydrogen-based e-fuels are often indicated as an option to abate greenhouse gas (GHG) emissions in sectors that cannot be directly electrified, such as aviation, shipping, chemicals, or the iron and steel industry [1,2]. E-fuel refers to liquid or gaseous fuels synthesized from hydrogen and carbon or hydrogen and nitrogen, the hydrogen being produced via water or steam electrolysis. Common e-fuels are e-methanol, e-methane, and e-ammonia and can be used directly or further processed into more advanced fuels or chemicals.

Some studies [1,3,4] assume that e-fuels are produced using a combination of wind and solar power. However, due to wind and solar power variability and the limited flexibility of the e-fuel synthesis plant [3,4], using only variable renewable electricity raises some technical and economic challenges. Indeed, using variable power requires large intermediate storage systems to avoid regular shutdowns that may reduce the performance and the lifetime of the fuel plant [4]. In addition, compared to a system with a constant electricity supply, the infrastructures (power supply, electrolyzer, fuel plant) need to be oversized to compensate the lower number of production at full load, which significantly increase the cost per fuel unit produced [5]. Therefore, fuel producers could be tempted to use an additional "available on-demand" power source such as hydropower, geothermal or biomass to increase the fuel plant full load hours and reduce the infrastructure size and costs. If these renewable resources are not available on site, it is likely that public grid would be used instead. In this case, the e-fuel GHG intensity depends on the Power-to-X (PtX) plant infrastructure's lifecycle emissions and the grid usage.

Some studies [6–9] are limited to cradle-to-gate operational emissions, and non-fossil electricity emissions are counted to zero, disregarding the emissions related to the construction and decommissioning of the infrastructures. When upstream emissions are counted [10], the potential fuel producer's "economic rational" behavior is not usually not considered, and the plant configuration assessed for lifecycle analysis (LCA) may be quite different from the one that the fuel producer would use to reduce its costs under specific technical constraints.

This study proposes a method that combines the technical feasibility, the economic profitability, and the GHG emissions accounting for e-fuel production. The emissions accounted are the ones related to the e-fuels plant infrastructure (renewable power supply, electrolyzer, intermediate storage, fuel plant) covering the complete life cycle of each component and the ones related to the grid electricity usage. All reviewed studies which include use of grid electricity [2,11] use an average grid emission factor derived from the country (or region) electricity mix, which does not consider the fuel plant's dynamic operation and the potential correlation between local renewable power availability and grid GHG intensity. This study considers "real-time" grid use emissions estimated from the hourly e-fuel electricity consumption and hourly grid production mix for a specific region. As a case study, we selected three different sites with remarkable renewable potential and liberalized electricity markets.

2. Method

The calculation of e-fuels GHG intensity is done in two steps. The first step is sizing the e-fuel plant, assuming that the plant owner looks for production cost minimization. This plant owner's economic rational behaviour is simulated using a least-cost optimization model minimizing investments and plant operation. The PtX system considered is presented in Figure 1.

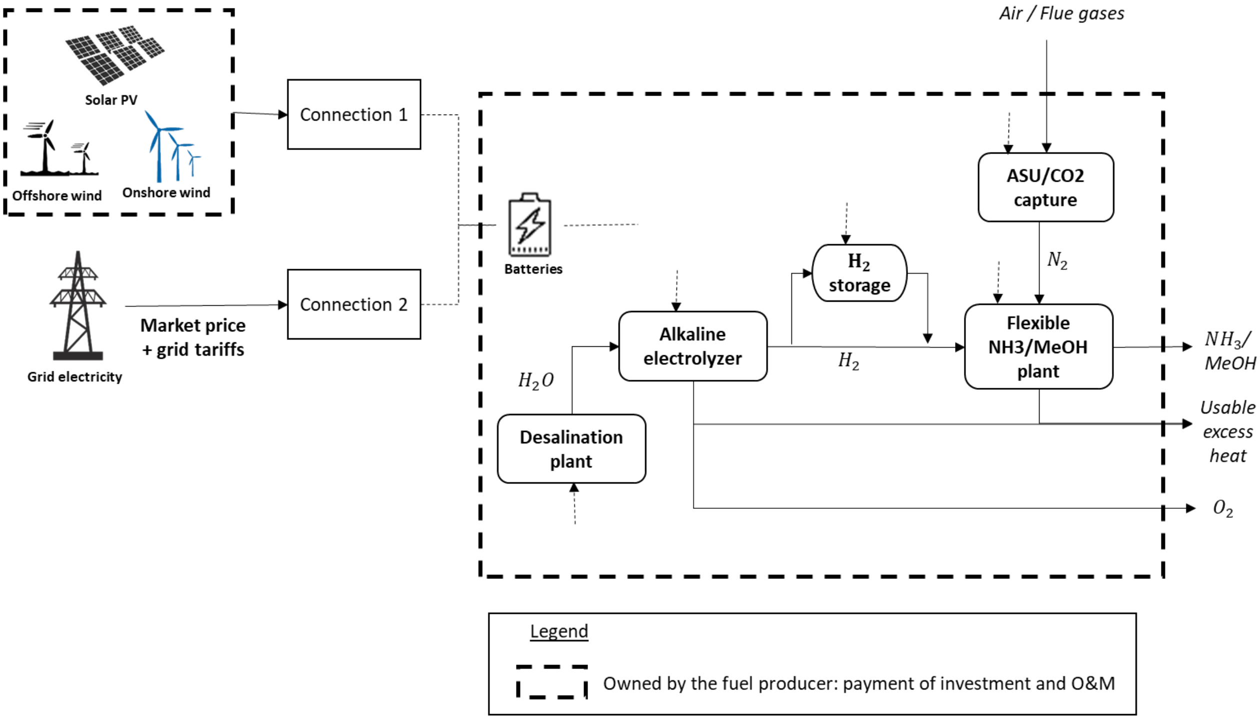

Fig. 1. PtX system description.

We consider that the fuel producer can choose to produce from renewable power only or use grid power or both depending on which configuration is the more economically advantageous. As a study case, three different sites with specific weather profiles are selected for this analysis: Arica in North Chile with a very high solar radiation but low wind power density, Esbjerg in Denmark with a high wind power density and low solar radiation, and finally Ceduna in Australia with good resources for both. We selected countries with a liberalized energy market, meaning that grid electricity price is variable (on an hourly basis) and potentially correlated to the wind and solar profiles depending on the country's energy mix. A fixed grid tariff is added to the spot market price to account for potential taxes and distribution fees. The data used to derive the optimal least-cost PtX plant design under realistic technical constraints are described in detail in [5] and [12]. The e-fuels studied are e-ammonia and e-methanol. The e-ammonia is produced through a Haber-Bosch process fed with electrolytic hydrogen and nitrogen extracted from the air via an air separation unit. The e-methanol is produced via CO_2 hydrogenation using electrolytic hydrogen and point source biogenic CO_2 as inputs. The main technical constraints considered in the model are the mass and energy balances, the minimal operation load of the different units, and the yearly production requirement fixed to 1 TWh of fuel per year (194 kt_{NH3}/y or 181 kt_{MeOH}/y). 1 TWh represents roughly the fuel consumption of the largest Triple E Mærsk ship (18 000 TEU capacity) for 230 days of operation cruising at 23 kts [13].

Then, once the least-cost plant design is determined based on techno-economic criteria and power supply profiles, related GHG emissions are accounted for, considering the plant infrastructures' life cycle and the grid usage. The emissions related to a potential grid re-enforcement or extension are not considered. The PtX plant is also assumed to be built in a site without displacing other activities (e.g., on a deserted area), so land-use-change emissions are not considered. The carbon footprint of each component of the e-fuel plant is derived from the EcoInvent consequential database 3.7.1 using the method IPCC 2013 with 100 years global warming potential (GWP) using global data or literature studies when the data is not available. The emissions are expressed in gCO2e/Capacity$_{installed}$ and include upstream and downstream emissions. The capacity installed represents the size of the different fuel plant components (expressed in tonne$_{output}$/h or MW) in the least-cost design, adapted for a yearly production of 1 TWh of fuel. Because the techno-economic model is based on one year of plant operation, the emissions are finally expressed in gCO2e/Capacity$_{installed}$/year, dividing the life cycle emissions by the infrastructure lifetime.

The grid usage emissions are calculated using the hourly regional grid production mix, including imports (in Chile, Denmark-DK1, and South Australia) and emissions of electricity production technologies. The emissions factors are taken from the EcoInvent consequential database 3.7.1 using the method IPCC 2013 with 100 years GWP in the region where the electricity is produced. Global data is used instead when data is unavailable for a specific region. The emission factors of the power generation technologies are expressed in gCO2e/kWh. The emissions factor data used in the model and the underlying assumptions are explained in further detail in [2].

All the time series of power supply profiles, grid prices, and hourly regional grid mix are based on real data from the same year (2019) to keep potential correlation between electricity price, weather, and hourly grid emissions.

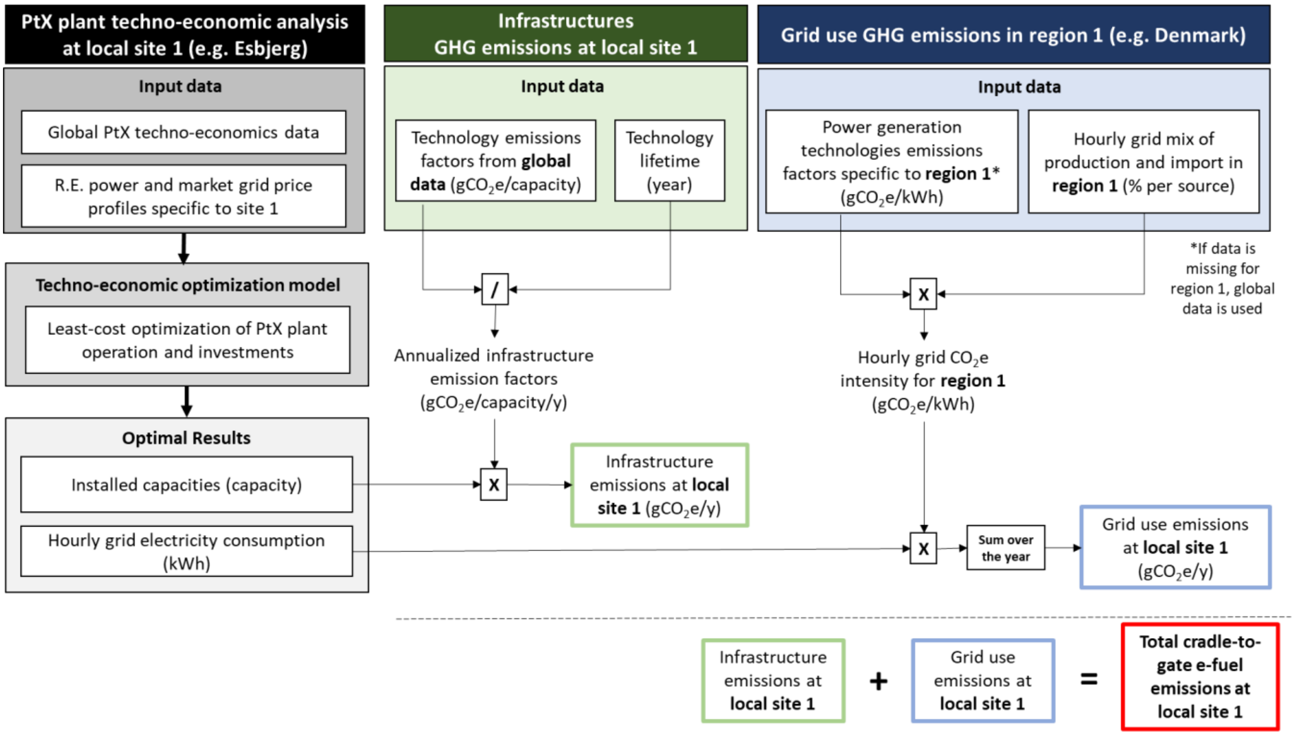

Fig. 2. Cradle-to-gate e-fuel carbon accounting method.

The use emissions related to e-methanol combustion are counted as zero, assuming that the carbon used in the hydrogenation process is biogenic and originates (for example) from the flue gases of a biomass-fired CHP plant. However, for large-scale applications, the availability of sustainable biomass remains questionable, and industrials may also choose to extract CO_2 from fossil point sources. Based on [14], The use emissions of e-ammonia combustion are also counted as zero, which may be optimistic given that ammonia combustion at the industrial scale has not been developed and studied extensively yet. Therefore, counting the use emissions as zero for e-ammonia and e-methanol can be interpreted as an optimistic scenario.

3. Results and discussion

3.1. Least-cost plant design and fuel production cost

Figure 3 shows the fuel production cost and the cost breakdown obtained in the least-cost configuration in the three selected sites. We differentiate the cases where a grid connection is possible and where the fuel production system is completely off-grid. When producing only with local renewable power (off-grid), large power supply, electrolyzer, and storage capacities are needed to operate the fuel above the minimum load and produce the required fuel quantity with limited full load hours. With a grid connection, the infrastructures do not need to be oversized, so the production cost is 15 to 30% lower. If the solar potential is high, the least-cost solution combines grid usage (usually during the night) and cheap solar power during the day. In Esbjerg, the 2019 grid prices were low to prefer local investments into wind power supply. The result is valid, assuming that the e-fuel plant is a marginal player with a limited impact on the market prices and that any grid infrastructure re-enforcement is not at the charge of the e-fuel producer. A more detailed analysis of the regulations, tariffs, and agreements between TSO and the e-fuel plant should be investigated for a real case study. Production costs are expressed in €/GJ_{fuel} where GJ_{fuel} represents the energy content of the fuels using the lower heating values of 18.6 GJ/kg for ammonia and 19.9 GJ/kg for methanol.

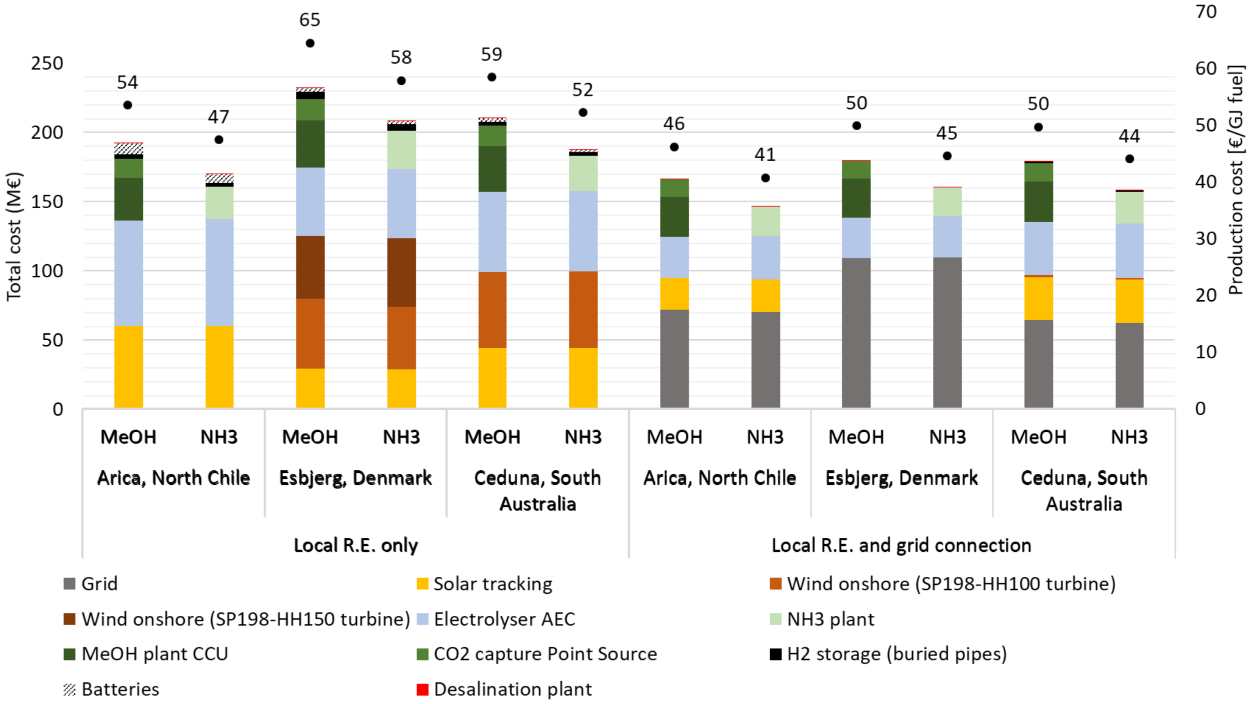

Fig. 3. Fuel production cost and cost break down in the cheapest configuration for 1 TWh of fuel produced per year. Grey ammonia and methanol costs are around 10 €/GJ fuel.

As shown in Figure 4, when a grid connection is possible, most of the power supply comes from the grid, the plant being grid powered during the night or when electricity prices are low. Therefore, in the least-cost configuration, the e-fuel emissions strongly depend on the grid CO_2e intensity. The rest of the power is mainly supplied with solar PV with one axis tracking if the solar potential is good enough. Without grid connection, solar PV is used in all the sites, no matter the solar potential. In sites where the wind potential is also significant, a mix of wind power and solar power is used.

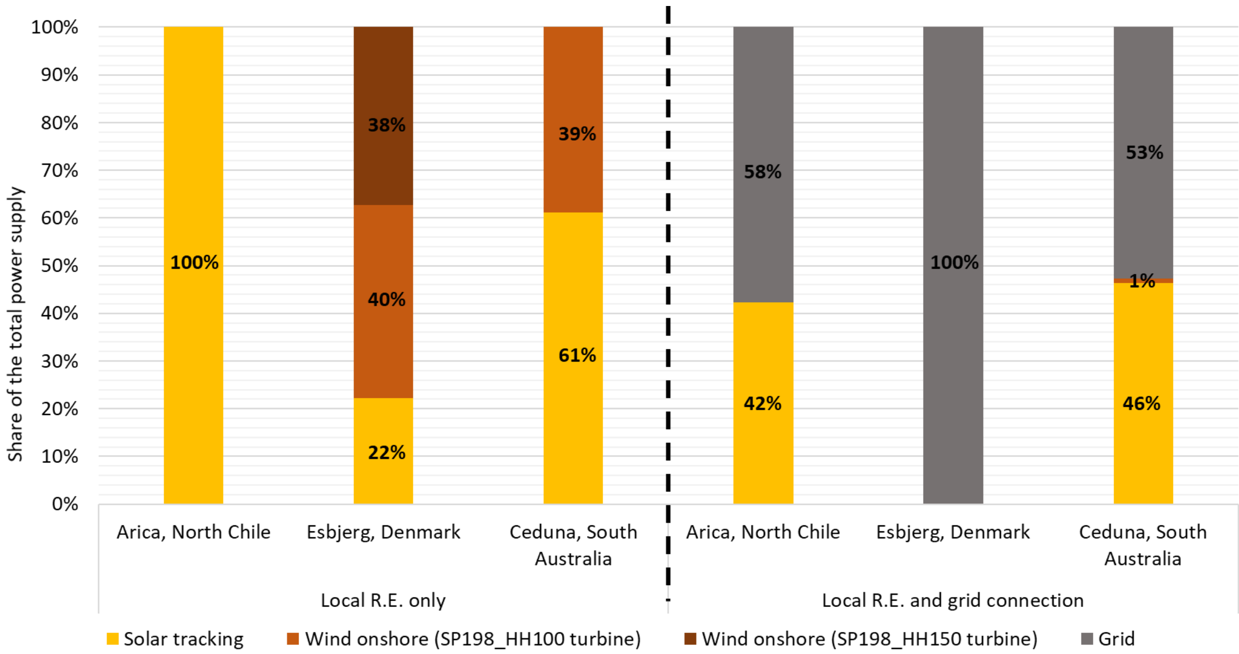

Fig. 4. Share of the total power supply per source in the cheapest configuration for ammonia production

3.2. E-fuel GHG emissions

The GHGs emissions related to fuel production are calculated using the method presented in section 2, and results are presented in Figure 5. We can see that with the regional grid mix of Chile, Denmark, and South Australia, using the grid electricity to reduce the production cost leads to very high e-fuel carbon intensity. With the share of grid electricity presented in Figure 4, the e-fuel GHG footprint is higher than the same fuel produced with natural gas (grey fuels), especially in Chile, where 60% of the grid electricity produced and imported originates from fossil sources (gas, coal, and oil) [15]. In Denmark, in 2019, only 20% of the electricity produced and imported originates from coal, gas or oil [16], explaining the relatively low GHG footprint compared to Chile even if only grid electricity is used. In South Australia, fossil electricity produced or imported represents 55% of the mix, most of it being natural gas [17]. With 47% of local renewable power supply, producing fuel in South Australia gives the lowest e-fuel GHG intensity while using the grid. However, life cycle emissions are only 25% lower than grey methanol (with a cost four times higher).

Producing the fuel off-grid requires larger infrastructure, which increases the upstream cradle-to-gate emissions but not substantially compared to a grid usage with the current electricity mix. Even if the production costs are 15 to 30% higher, producing the e-fuel with local renewable reduces the GHG footprint 4 to 8 times. These conclusions are valid, assuming that land-use change emissions are null, meaning that no natural carbon sink is displaced when installing the power plant. To produce 1 TWh of fuel per year (enough for 230 days of operation of a Triple E containership at full speed), the least-cost off-grid solution in Arica suggests that 900 MW of solar PV should be installed, so around 16.2 km^2 counting 18 000 m^2 per MWp installed [18]. The carbon footprint associated with the batteries, electrolyzer, fuel plant, and storage system infrastructures is not significant compared to the emissions related to the power supply (wind and solar PV) so they barely appear in Figure 5.

In all cases, producing methanol or ammonia gives very similar life cycle GHG intensity assuming that emissions related to fuel use are null in both cases.

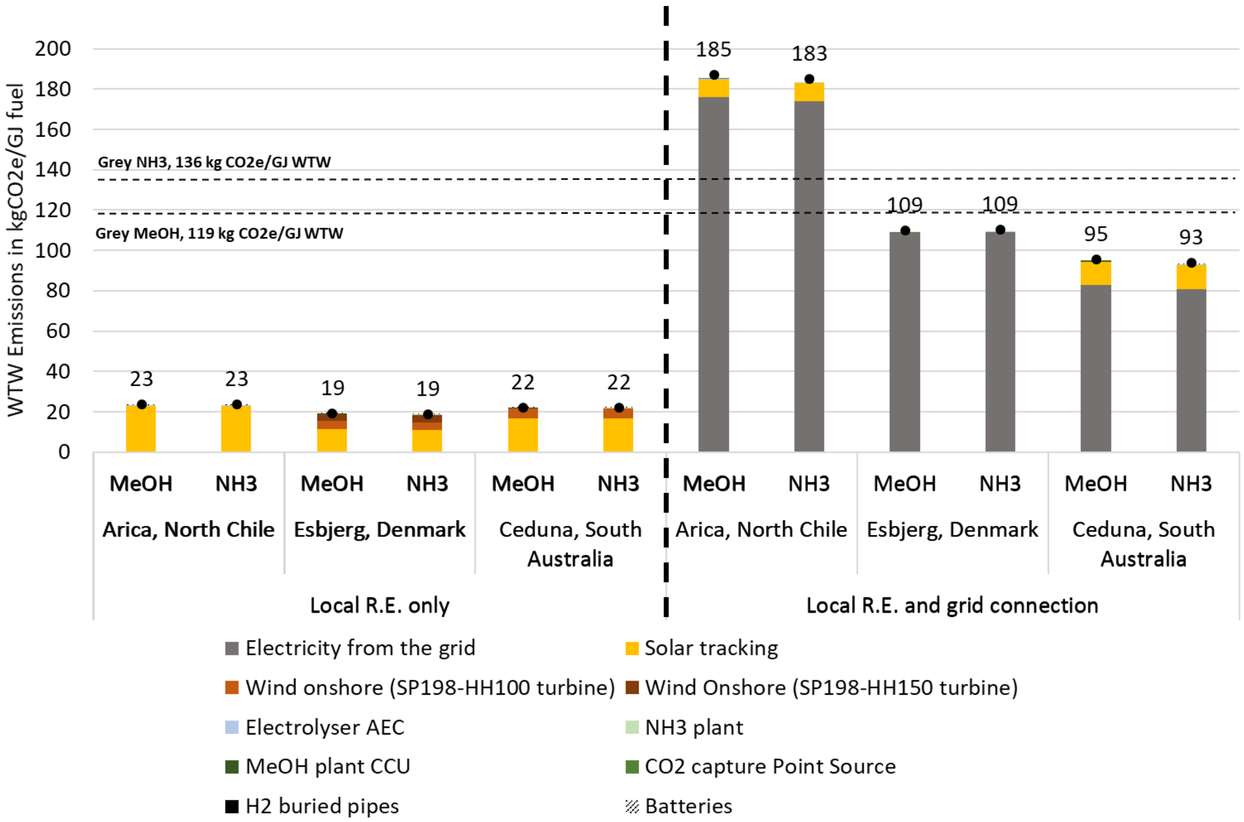

Fig. 5. Upstream and operational cradle-to-gate CO2e emissions for e-fuels.

Grey methanol or ammonia refers to fuels produced from natural gas using steam reforming without carbon capture. The emissions of grey methanol and ammonia are calculated adding the upstream emissions from EcoInvent data base 3.8 and the combustion emissions derived from the carbon content of each fuel.

4. Conclusion

We developed a method to quantify the GHG emissions caused by e-fuel production while minimizing the fuel production cost. The e-fuel plant is powered using local renewable power with the possibility to add a grid connection if it reduces the production cost. We studied three regions with high solar or wind resources. The plant operation and investments are optimized for each local site to minimize the production according to weather profiles and electricity prices. Life cycle GHG emissions are estimated considering the least-cost plant design and operation. The cradle-to-gate emissions account for the complete lifecycle of infrastructures and the grid usage emissions, calculated hourly, given the regional production and import electricity mix. We assumed that use phase emissions are negligible for e-fuels. With the data set used, the main conclusions from this analysis are:

- If the solar resource is high, like in South Australia and North Chile, the least-cost configuration uses local solar PV 1-axis tracking and grid power. In the cheapest configuration, the grid provides more than 50% of the electricity, usually at night. In Denmark, given the assumptions taken for wind power cost and grid prices, using only grid electricity is the cheapest option. In this case, the production cost is still 4 times higher than 2019 grey ammonia or methanol price.
- Compared to off-grid solar and wind-powered e-fuel plant, using a grid connection reduces the production cost by 15-30% but increase the e-fuel carbon footprint from 4 to 8 times.
- With the current hourly grid carbon intensity in the selected regions, using the grid in a cost minimization perspective produces e-fuels with life cycle emissions between 93 and 185 gCO_2e/MJ, which is on the same range as grey methanol and ammonia emissions.
- In the off-grid setup, most of the emissions originate from the solar PV and wind infrastructures. The other components of the fuel plant have a limited impact on the carbon footprint. The life-cycle emissions are lowered to between 19 to 22 gCO_2e/MJ, which is 6 times lower than grey methanol.
- If the carbon used to produce methanol is biogenic, producing e-methanol or e-ammonia leads to similar life cycle emissions for the routes considered.

As we concluded, using backup power like grid electricity can be beneficial to reduce the production costs, the space requirement and facilitate plant operation but can lead to very high GHG emissions. However, with a different approach than cost minimization alone, the benefits of using the grid (or any other backup power) may also be combined with controlled GHG emissions. Further work could focus on the effect of an additional carbon tax on the grid electricity, restricted usage depending on the hourly GHG intensity or the use of Power Purchase Agreements, and identifying the best trade-off between technical feasibility, space requirement, cost, and e-fuel emissions. The usage of other types of "available on demand" backup power, which would limit the cost and infrastructures size, can also be investigated. Other environmental impacts such as human toxicity, minerals and metal use, or land-use change could also be investigated as they may be significant considering batteries, electrolyzers and PV panels manufacturing and the space required for the PtX plant.

If the results and the conclusion drawn in this study are sensitive to the input data and may differ slightly with different techno-economic or emissions factors assumptions, some clear recommendations always remain valid:

- Off-grid production ensures relatively low life cycle e-fuel emissions involving higher production costs and space requirements.
- With the current electricity mix of most countries, using the grid electricity with a cost minimization perspective without controlling the quantity and the origin of electricity is not an option to produce "green" e-fuels.

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