Appendix to "Technoeconomic evaluation of the electrochemical production of renewable ethylene oxide from fluctuating power sources and CO_2"

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A. GIS-BASED BIOGENIC CO_2 POTENTIAL ANALYSIS FOR EUROPE

The data of biomethane upgrading plants was gathered from the 2018 biomethane map and its associated database prepared by Gas Infrastructure Europe (GIE) and European Biogas Association (EBA). The biomethane capacity information was used to calculate the yearly CO_2 production for 8,000 operating hours and 40%-vol. CO_2 in the raw biogas. An detailed information of the location of the biomethane plants is given in [44] and its updated version in [45]. Most of the biomethane plants are located in Germany, followed by France and the UK. The data of bioethanol production sites was gathered from EPURE and company websites. The produced CO_2 amount was either taken from company websites directly (as at some plants the CO_2 already is utilized/sold) or calculated. Latter calculations are based on the available information on bioethanol production as well as stoichiometric calculations, based on chemical Eq. (A.1):

$$C_6H_{12}O_6 \rightarrow 2\ C_2H_5OH + 2\ CO_2 \qquad \textbf{Eq. (A.1)}$$

This means that1 kg of ethanol produced leads to a theoretical CO_2 potential of ~ 0.96 kg. See also Rodin et al. [38] for further information on the CO_2 potentials in Europe. For some companies, neither ethanol/biomethane nor CO_2 production was available, only the location. Despite this, these locations were included in the QGIS analysis as well. The most important data for the subsequent data analysis in QGIS were the location and CO_2 production capacity in t/a (see Fig. (A.1)).

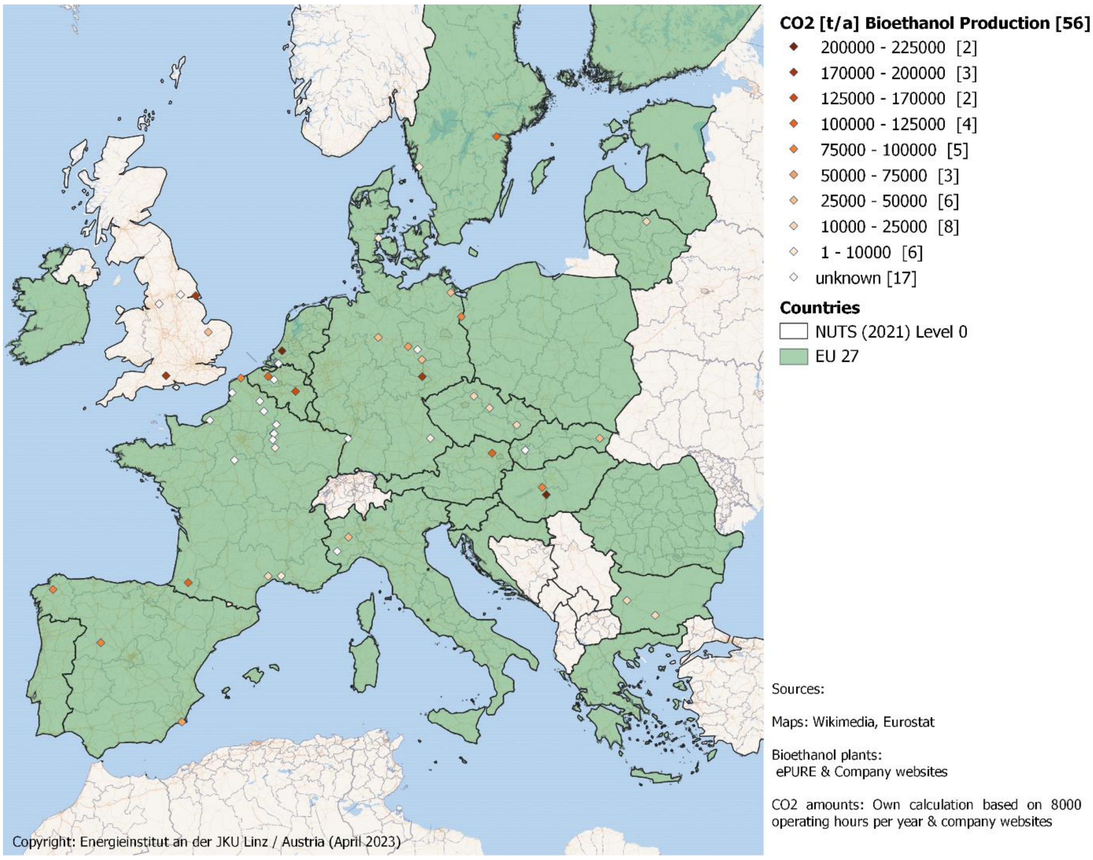


Fig. (A.1) Exemplary results of the GIS processing of existing bioethanol plants. The color indicates the theoretical CO_2 potential. No claim to completeness. Source: based on data from [43] and derived company websites.

B. Localization of large wind and PV plants

In total, ~3619 wind farms in operation from 1-5 MW were identified. Additionally, ~6055 wind farms in operation with 5-600 MW were localized. Most of them are located in Germany, Belgium, Denmark followed by France, the UK, Ireland, and Spain (see Fig. (B.1) for an overview). In the case of parks that were partially shut down or were under construction, only operational units were included.

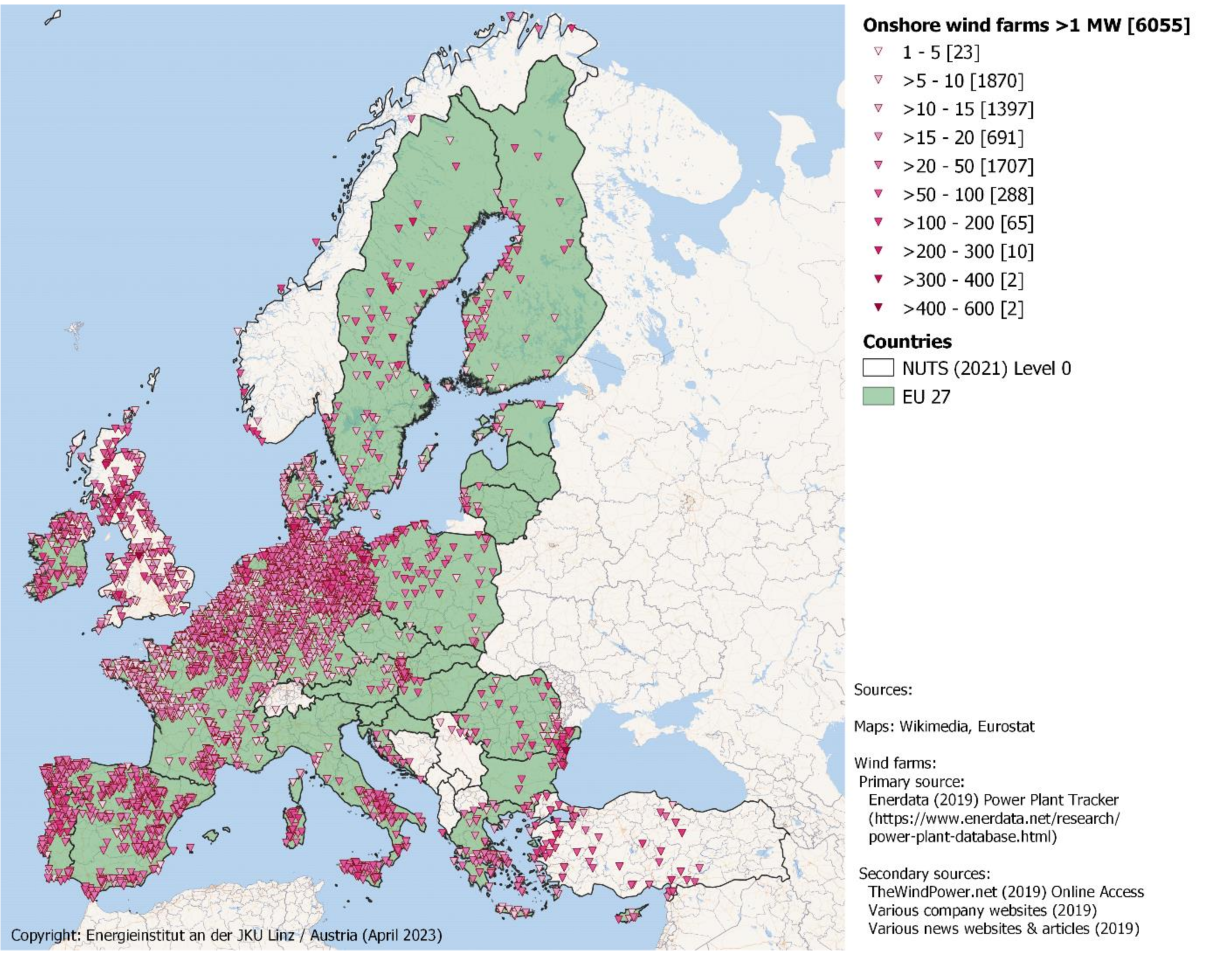


Fig. (B.1) Exemplary results of the GIS processing of existing onshore wind farms 5 to 600 MW. Color indicates the rated power. No claim to completeness. Source: based on data from [46,106] and derived websites (companies, newspaper articles i.a.).

In total, approximately 3174 PV plants in operation with a capacity of 1–230 MW were identified across Europe. Most of these are located in the UK (see Fig. (B.2) for an overview).

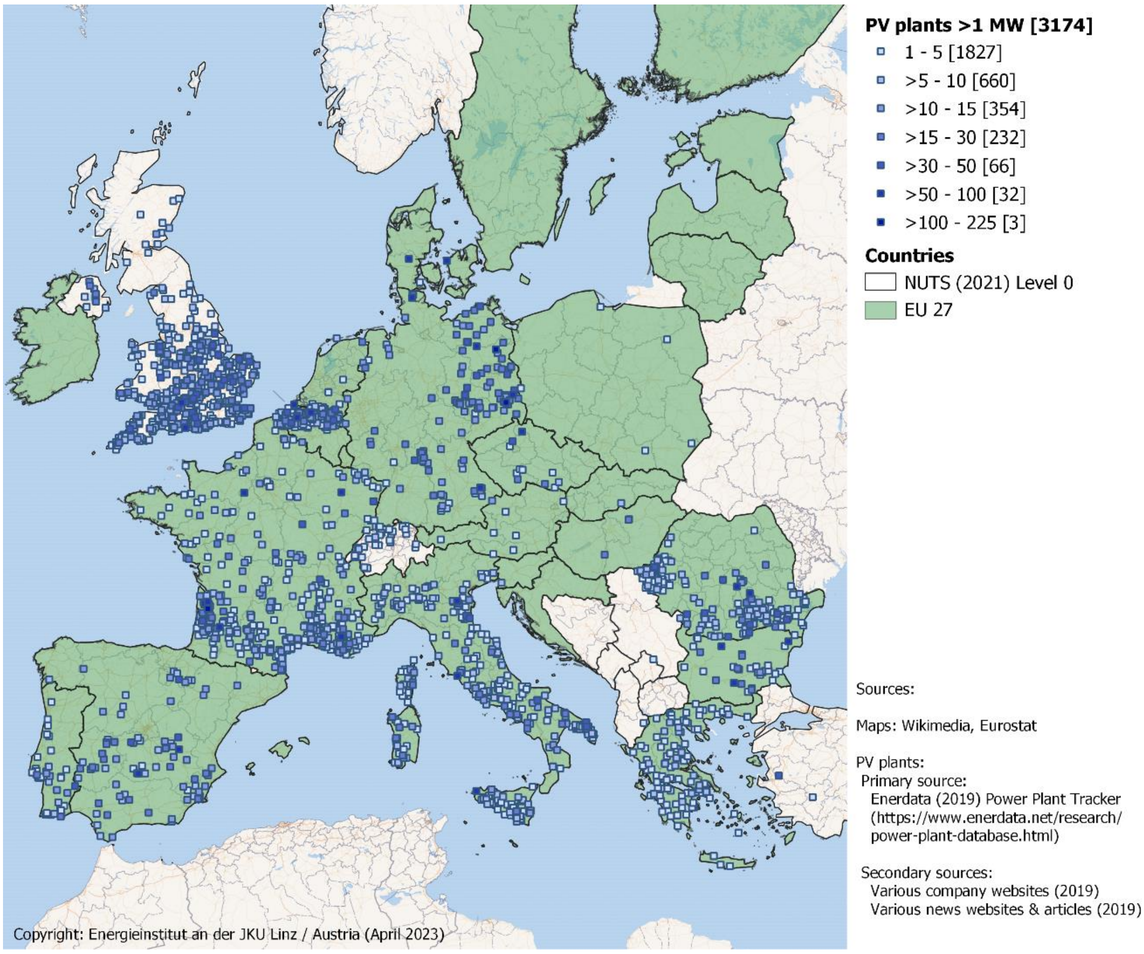


Fig. (B.2) Exemplary results of the GIS processing of existing PV plants 1 to 230 MW. The color indicates the rated power. No claim to completeness. Source: based on data from [46] and derived websites (companies, newspaper articles i.a.).

C. CONSIDERATION OF EXISTING REFINERIES AND ETHYLENE PIPELINES

As ethylene and ethylene oxide are important bulk chemicals, there is a wide European infrastructure of producers and consumers, as well as distribution pathways, such as pipelines. Fig. (C.1) provides a rough overview of the existing and planned pipelines, as well as some large production/utilization sites. As the information was gathered through desk research from a variety of sources, there is no claim to completeness or timeliness of the information, e.g., some of the "Vision 2020" pipelines are likely to have been built or abandoned. Nevertheless, the location of pipelines and large facilities that produce/consume ethylene (oxide) allowed a reduction in the number of ideal electrochemical production plant locations.

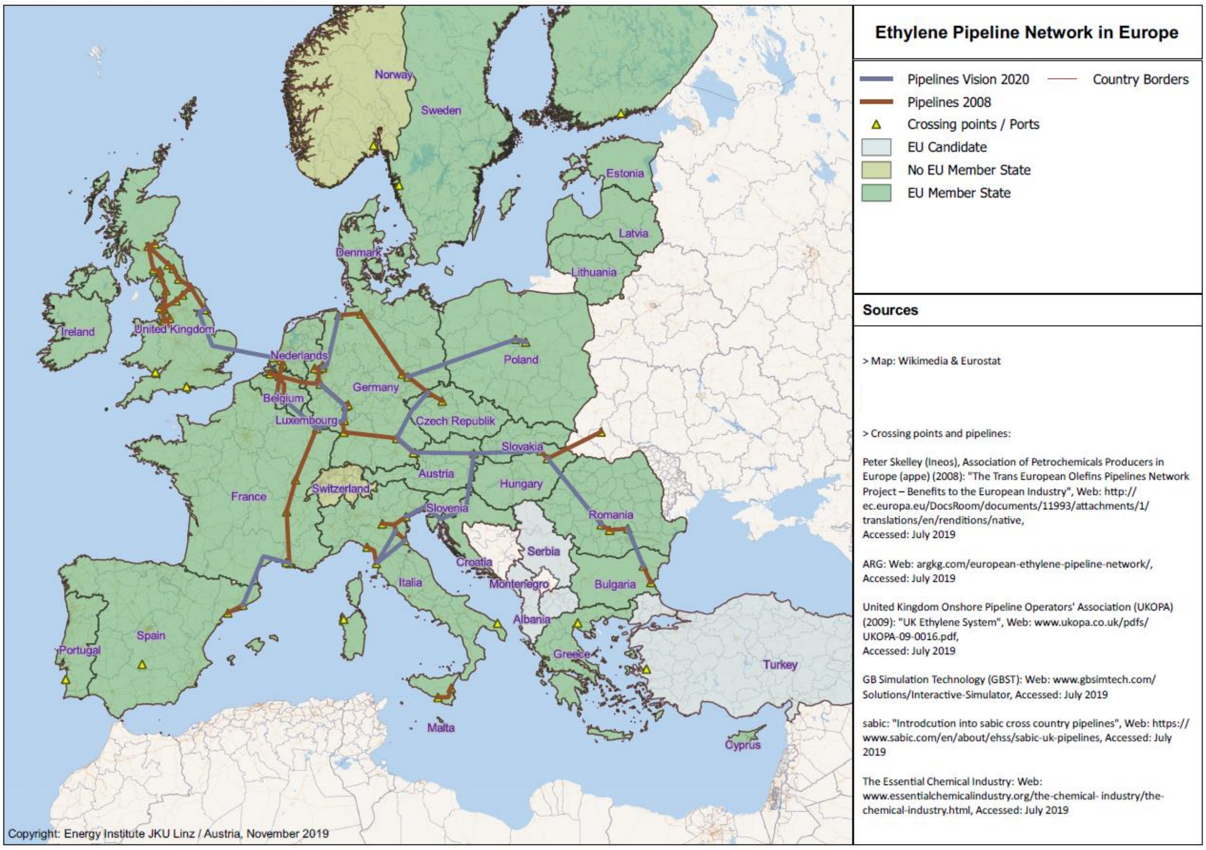


Fig. (C.1) Exemplary results of the GIS processing of ethylene pipelines across Europe as well as their crossing points and large chemical industry being related to ethylene (yellow triangles). No claim to completeness. Source: based on [64–70,107,108].

D. Detailed Data on Case Study Sites

D.1 Austrian Site

Fig. (D.1) Location of the biomethane plant Bruck/Leitha and wind farms and C_2H_4 pipeline in close proximity based on Table (D.1). Wind icon [109]. Map data ©2020 Google

Table (D.1) Overview of CO_2 and power sources in Bruck/Leitha, Austria. Sources: [44,46,71–73,110–112]

CO_2-source		**Matched wind power plants**		
Plant name	Biogasanlage Bruck/Leitha	**Plant name**	Bruck an der Leitha (Windpark Bruck)	Bruck an der Leitha - 2 (Bruck-Göttlesbrunn)
Coordinates	48.031866, 16.821901	**Coordinates**	48.03376, 16.72678	48.04036, 16.71316
Year	2004 (2014: biomethane upgrading)	**Year**	2000	2015
Substrate	vegetable + animal residues (+ interim crops)	**Installed Power [MW]**	9	21
Separation Technology	gas pre-treatment + three-stage membrane system	**Annual energy generation (simulated) [MWh/a]**	21101	75234
Biomethane Feed-in Capacity [m^3/h]	500	**Annual energy generation (literature) [MWh/a]**	15000	51000
CO_2 amount (calculated) [t/a]	5280			
CO_2 amount (literature) [t/a]	3366			

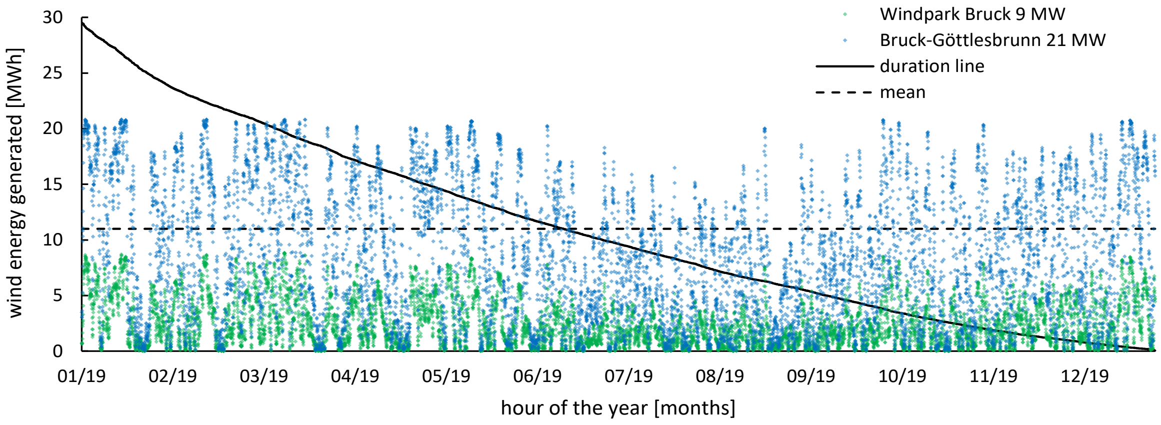


Fig. (D.2) Power generation of the RES considered in the Austrian case study. Data source: simulated with Renewables.Ninja [71] based on wind farm data from VERBUND [72,73]

D.2 GERMAN SITE

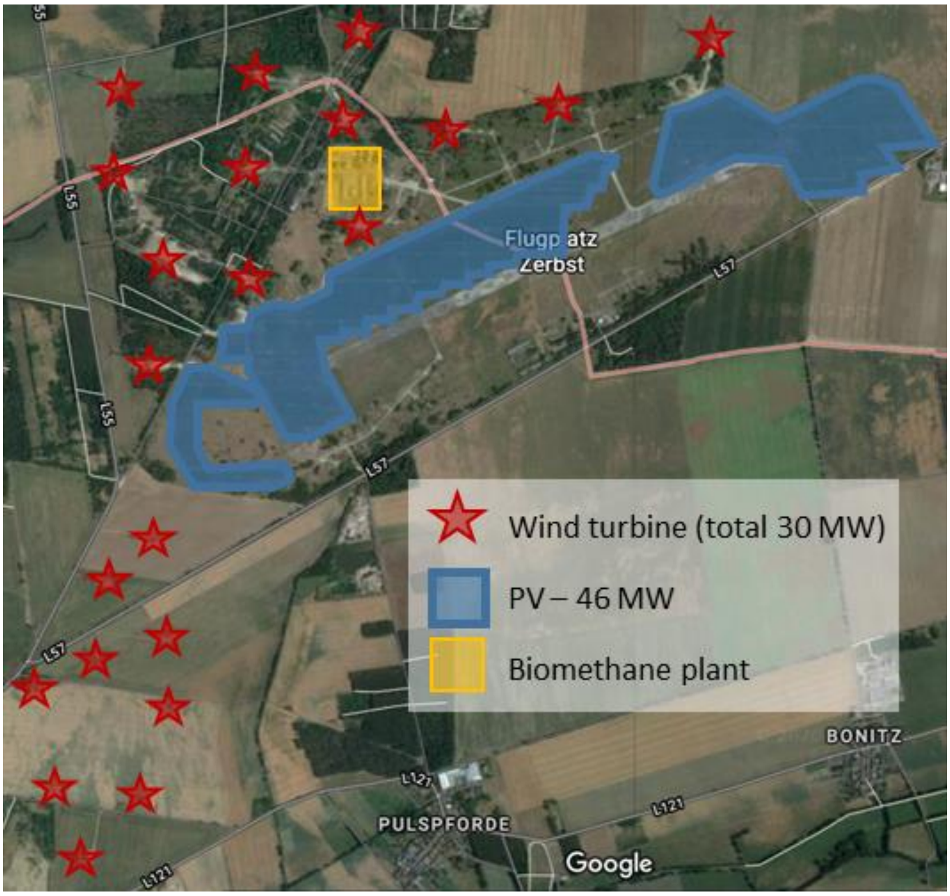


Fig. (D.3) Location of the biomethane plant Zerbst within Energy Park Zerbst and the close-by wind farm and solar plant, which are also part of Energy Park Zerbst based on Table (D.2). Map data Google et al. [113,114]

Table (D.2) Overview of CO_2 and power sources in Zerbst, Germany. Sources: [44,46,71,75,115–118]

CO_2-source		**Matched power plants**	**Wind power**	**Solar power**
Plant name	Energiepark Zerbst	**Plant name**	Zerbst 5 (Windpark Zerbst)	Zerbst
Coordinates	52.003302, 12.133536	**Coordinates**	51.984869, 12.119544	51.998757, 12.134478
Year	2014	**Year**	2015	2011
Substrate	Energy crops	**Installed Power [MW]**	30	46
Separation Technology	Water scrubbing	**Annual energy generation (simulated) [MWh/a]**	57658	52000
Biomethane Feed-in Capacity [m^3/h]	770			
CO_2 amount calculated [t/a]	8131			

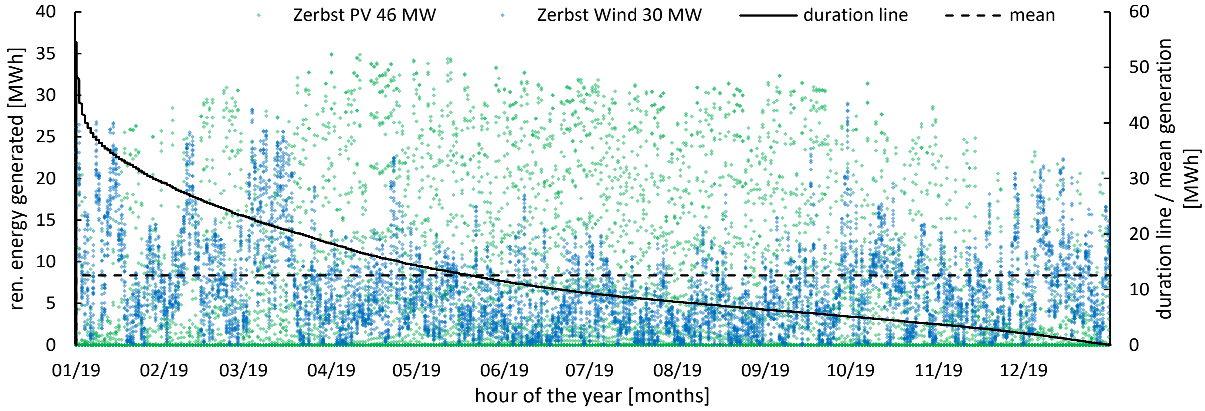


Fig. (D.4) Power generation of the RES considered in the German case study. Data source: wind power simulated with Renewables.Ninja [71], solar power simulated with PVGIS [75] based on wind and solar plant data from [115–118]

D.3 UNITED KINGDOM SITE

Fig. (D.5) Location of the biomethane plant Gore Cross close to Arreton and close by PV plants based on Table (D.3). PV icon [119]. Map data ©2020 Google

Table (D.3) Overview of CO_2 and power sources on the Isle/Wight, UK. Sources: [44,46,75,77,120–123]

CO_2-source		**Matched PV plants**				
Plant name	Gore Cross	**Plant name**	East Fairlee	Fieldscale	Grange Farm	Ventnor Road Solar Park
Coordinates	50.675146, -1.253390	**Coordinates**	50.715837, -1.274390	50.657023, -1.235434	50.712930, -1.261002	50.641604, -1.199894
Year	2014/2015	**Year**	2015	2016	2015	2013
Substrate	Energy crops	**Installed Power [MW]**	7.3	10.6	6	4.8
Separation Technology	Membrane technology	**Annual energy generation (simulated) [MWh/a]**	6987	9769	5742	4640
Biomethane Feed-in Capacity [m^3/h]	580					
CO_2 amount (calculated) [t/a]	6336					
CO_2 amount (literature) [t/a]	6900					

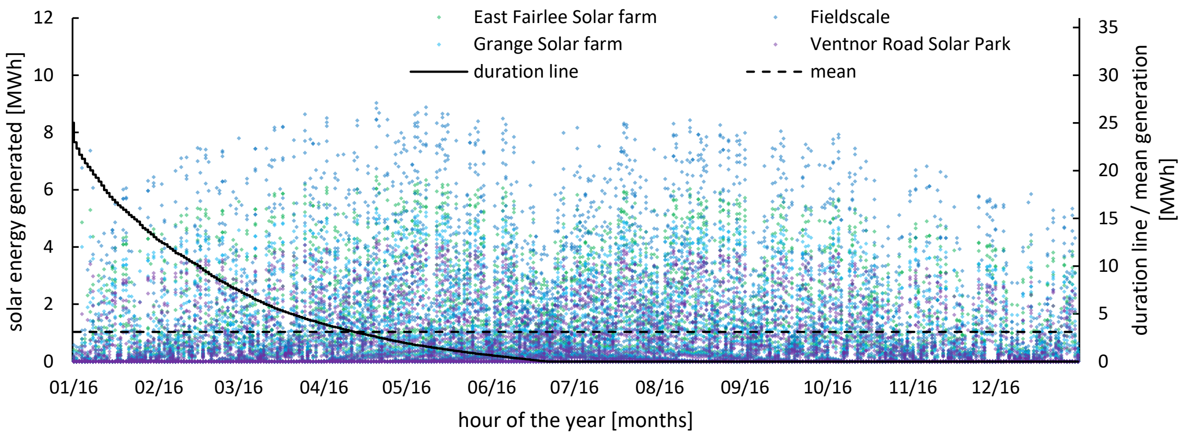


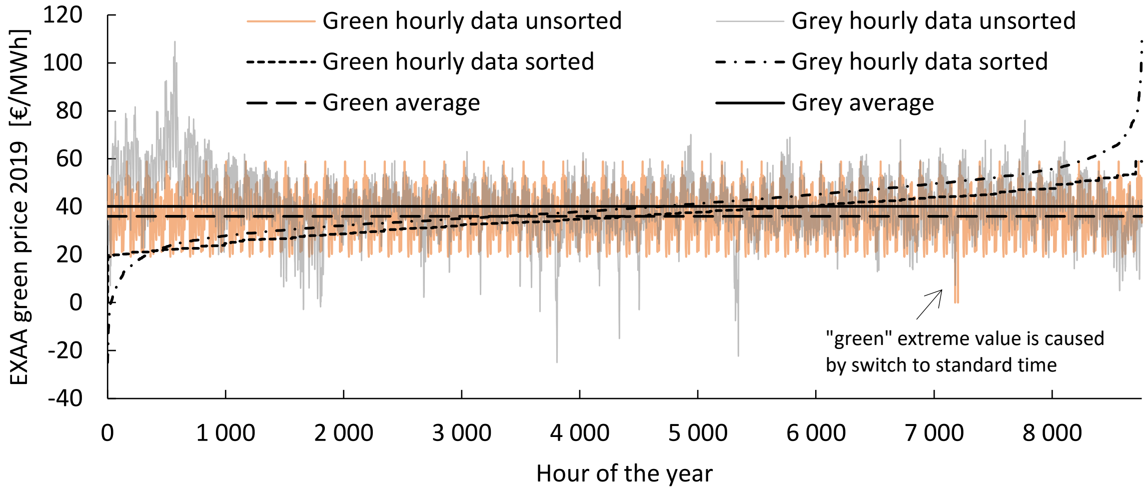
Fig. (D.6) Power generation of the RES considered in the UK case study. Data source: solar power simulated with PVGIS [75] based on solar plant data from [120,122,123]

E. COST CONVERSION FACTORS

Table (E.1) Calculation factors used for cost conversion between sources of different currencies and publication dates

Conversion	Factor
Currency	
USD to EUR (2010)	0.755
USD to EUR (2013)	0.779
USD to EUR (2018)	0.847
USD to EUR (2021)	0.846
Inflation	
2010 to 2021	1.15
2013 to 2021	1.09
2018 to 2021	1.04

F. ELECTRICITY SPOT MARKET PRICES



Green electricity
Average: 36.01 €/MWh
Average deviation: +/- 7.16 €/MWh
Min: 0 €/MWh
Max: 58.93 €/MWh

Grey electricity
Average: 40.16 €/MWh
Average deviation: +/- 9.29 €/MWh
Min: -25 €/MWh
Max: 108.99 €/MWh

Fig. (F.1) Hourly EXAA green and grey electricity spot prices based on [86]

G. GHG FACTORS

Table (G.1) Overview of fossil reference products' GWPs.

GWP fossil reference products	Value	Unit	Source
Ethylene	1.28	$kg_{CO2eq.}/kg_{C2H4}$	[124]
Ethylene oxide (EO)	1.51	$kg_{CO2eq.}/kg_{EO}$	[125]
Hydrogen peroxide	1.68	$kg_{CO2eq.}/kg_{H2O2}$	[126]
Hydrogen	7.77	$kg_{CO2eq.}/kg_{H2}$	[127]
Methane	0.578	$kg_{CO2eq.}/kg_{CH4}$	[128]

H. LEVELIZED COST OF PRODUCTION

To estimate potential production costs, the levelized cost of production ($LCoP$) was chosen as an appropriate specific indicator, calculated, and compared to similar evaluations performed in other PtX assessments [53]. The approach is similar to the levelized cost of electricity ($LCoE$) method, which is commonly used for electricity production cost evaluation [54]. The assessment considers a full year of operation in which the total annual cost is calculated using the annuity method [55].

$$LCoP = \frac{-A + \sum_i C_{var,i}}{M_{out}} \qquad \textbf{Eq. 1}$$

where

A = annuity of the fixed total annual payments, such as capital- and operation-related costs

M_{out} = total annual product mass-related output

C_{var} represents variable cost and revenues that depend upon the corresponding material and energy streams, and are, thus, related to the annual time of operation and potential variable load conditions, such as part-load efficiencies. These include demand-related cost for resources such as electricity, CO_2, and H_2O, as well as potential byproduct sales.

For the calculation of Ac and further factors, refer to Appendix H.

The capital-related annuity, defined in Eq. 2, considers the investment costs of the main equipment of the plant and the future cost of the expected replacement of individual components within the observation period.

$$A_C = (I_0 + I_1 + \cdots + I_n - R) \cdot a \qquad \textbf{Eq. 2}$$

where

I_0 = initial investment cost

I_1 ... I_n = first to nth replacement investments

R = residual value of the plant at the end of the observation period

a = annuity factor

The cash values of replacement investments and residual values are calculated from the interest rate factor $q = 1 + i$ (where i is the interest rate) and the presumed depreciation period T_N:

$$I_n = \frac{I_0}{q^{n \cdot T_N}} \qquad \textbf{Eq. 3}$$

$$R = I_0 \cdot \frac{(n+1) \cdot T_N - T}{T_N \cdot q^T} \qquad \textbf{Eq. 4}$$

The annuity factor a in Eq. 2 is calculated based on the interest rate factor and observation period, as follows in Eq. 5:

$$a = \frac{q^T \cdot (q-1)}{q^T - 1} \qquad \textbf{Eq. 5}$$

As only investment cost for the main equipment are directly included in the capital-related annuity, additional cost, such as those for engineering, construction, and commissioning of the plant, were considered in the form of appropriate overhead factors [56].

The annuity of operation-related cost (maintenance and insurance) was considered as fixed factor related to the initial investment I_0 and was likewise multiplied by annuity factor a.