HYDROGEN IN THE CHEMICAL INDUSTRY

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Markets and market drivers for carbon-neutral chemicals and fuels

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MARKETS, DRIVERS, REGULATIONS

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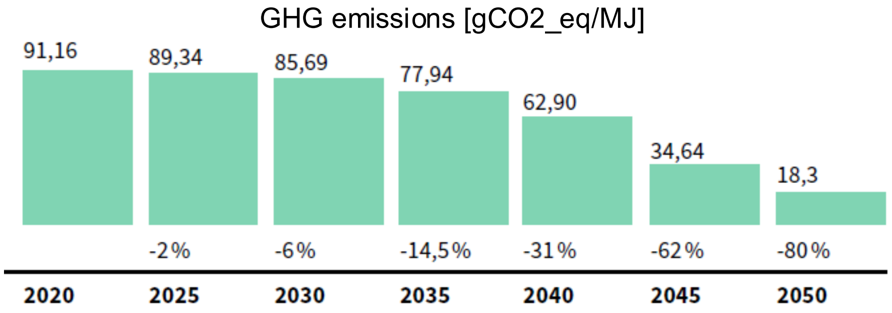
European demand for fuels with reduced GHG emissions

European regulations (ReFuelEU) require the reduction of greenhouse gas emissions for different fuels

- Greenhouse gas reduction pathways have to be fulfilled in order to avoid fines
- Certain quota are specified for the drop-in fractions of different production routes

Reduction of GHG emission for maritime fuels



NOW-Factsheet_FuelEU-Maritime.pdf

Quota for synthetic air fuels (SAF)

Jahr	Beimengungsziel	Davon PtL
Ab 2025	2 %	-
Ab 2030	6 %	-
2030–2031	-	1,2 % [2]
2032–2034	-	2,0 % [3]
Ab 2035	20 %	5 %
Ab 2040	34 %	10 %
Ab 2045	42 %	15 %
Ab 2050	70 %	35 %

Quellen: Agora Verkehrswende and International PtX Hub, https://www.agora-verkehrswende.de/fileadmin/Projekte/2024/E-Fuels-im-Luftverkehr_EN/111_Defossilising_Aviation_with_e-SAF.pdf; Finish Transport and Communications Agency, Finland's https://www.theglobaleconomy.com/rankings/jet_fuel_consumption/

MARKETS, DRIVERS, REGULATIONS

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European demand for fuels with reduced GHG emissions

Possible maritime fuel demand

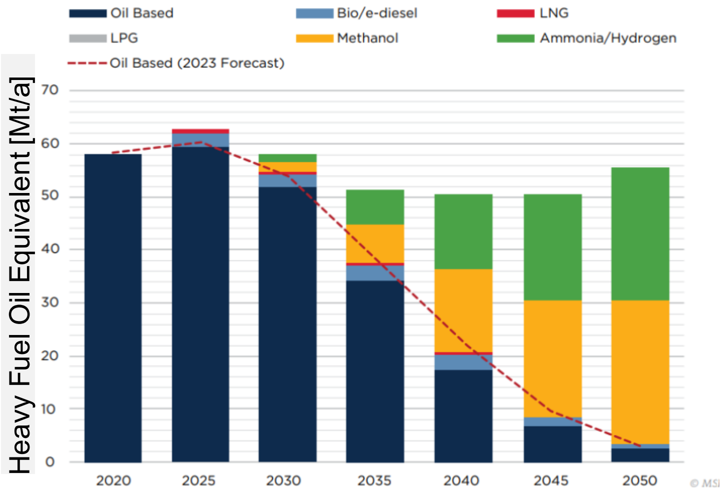
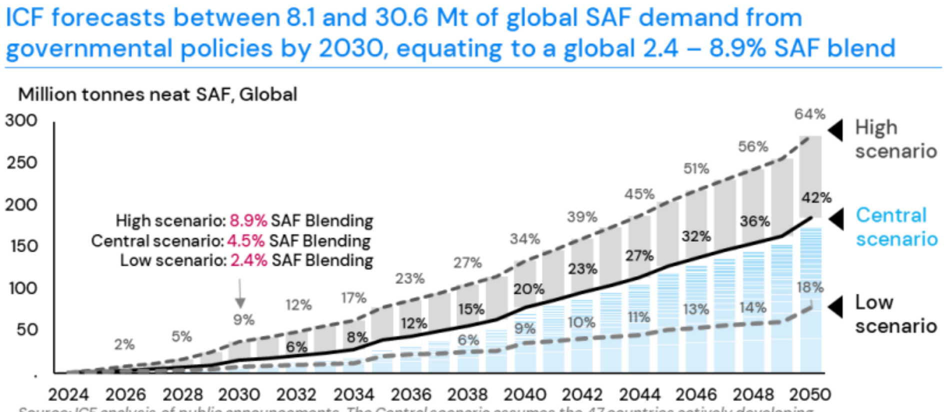


Figure 2.10: Fuel mix for dry bulk carriers.

ABS Outlook 2024: Fossil fuel use declining but will remain present - SAFETY4SEA

Possible aviation fuel demand



Source: ICF analysis of public announcements. The Central scenario assumes the 47 countries actively developing policies implement these at a reasonable level, including the EU, UK, US, Canada, Brazil, Australia, Japan, Malaysia, Indonesia, Singapore, India, China, and others. The Low scenario only includes countries with policies in-place, such as the EU, UK, US, and Singapore. The High scenario assumes global targets, such as CAAF/3 are met through initiates in additional countries. ICF notes that this is a forecast based on present-day assumptions, and higher volumes may be achieved if aspirations and resulting policies accelerate over the coming years.

EU_Industial_Strategy_SAF_Report_A4E_ACI_ARC_ASD_ERA_GAMA_January 2025.pdf

MARKETS, DRIVERS, REGULATIONS

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European production and import volumes of selected bulk chemicals

		2024		
	TIME	Production	Imports	TOTAL
	FREQ (Labels)	Mt/a	Mt/a	Mt/a
20141130	Ethylene	11.67	1.16	12.83
20141140	Propene (propylene)	10.08	0.23	10.30
20141150	Butene (butylene) and isomers thereof	2.44	0.00	2.44
20141160	Buta-1,3-diene and isoprene	2.26	0.01	2.27
20141223	Benzene	5.02	0.53	5.55
20141225	Toluene	1.05	0.04	1.10
20141243	o-Xylene	0.17	0.18	0.35
20141245	p-Xylene	0.70	0.18	0.88
20141247	m-Xylene and mixed xylene isomers	0.80	0.00	0.80
20142210	Methanol (methyl alcohol)	0.78	6.32	7.10
20145260	Melamine	0.15	0.17	0.33
20146111	Methanal (formaldehyde)	2.44	0.02	2.45
20153130	Urea containing > 45 % by weight of nitrogen	2.09	0.32	2.42
20153180	Urea containing <= 45 % by weight of nitrogen	1.45	1.42	2.87

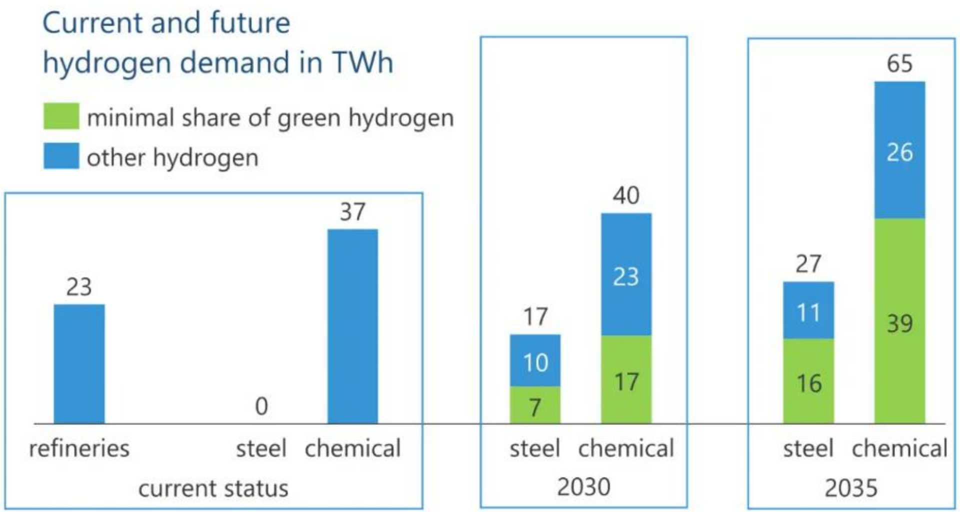
Dataset: DEF_DISS_DS-056121_ [ds-056121$defaultview]

MARKETS, DRIVERS, REGULATIONS

RFNBO demand for the production of chemicals with reduced GHG emissions

The EU's **Renewable Energy Directive III (RED III)** specifies targets for the use of RFNBOs (renewable fuels of non-biological origin) instead of fossil hydrogen

- 42 % “RFNBO-H2” in 2030
- 60 % “RFNBO-H2” in 2035



ffe.de/en/publications/consequences-of-the-red-iii/

MARKETS, DRIVERS, REGULATIONS

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Requirements on “carbon” for the production of chemicals with reduced GHG emissions

OPTION	Option 1: »Fossil option«	Option 2: »Direct Air Capture option«	Option 3: »Biogenic option«	Option 4: »RFNBO option«	Option 5: »Geological option«
THINGS TO CONSIDER	• must stem from an activity listed under this Directive 2003/87/EC Annex I • must have been taken into account upstream in an effective carbon pricing mechanism • only a viable option for receiving the deduction until 2041 (2036)	• no relevant additional criteria other than the accounting of emissions related to electricity and other processes used for the capturing process	• must comply with sustainability and GHG saving criteria (RED II Article 29) • did not receive emissions credits from CO_2 capture and replacement under the RED II framework	• fuel from which the CO2 is derived, must be regonised as RFNBO	• must have been previously released naturally

Relevant for all activities:
- Emissions from capturing, transportation and storage processes must be added in any case
- CO_2 must not stem from a fuel that is deliberately combusted for the specific purpose of producing the CO_2
- CO_2 must not have received an emissions credit under other provisions of the law

Source: GIZ, Identification of suitable carbon as feedstock for PtX products to be exported to Europe, June 2024, Link,

Production of “green methanol” via the synthetic route in Austria

SYNTHETIC CARBON NEUTRAL CHEMICALS

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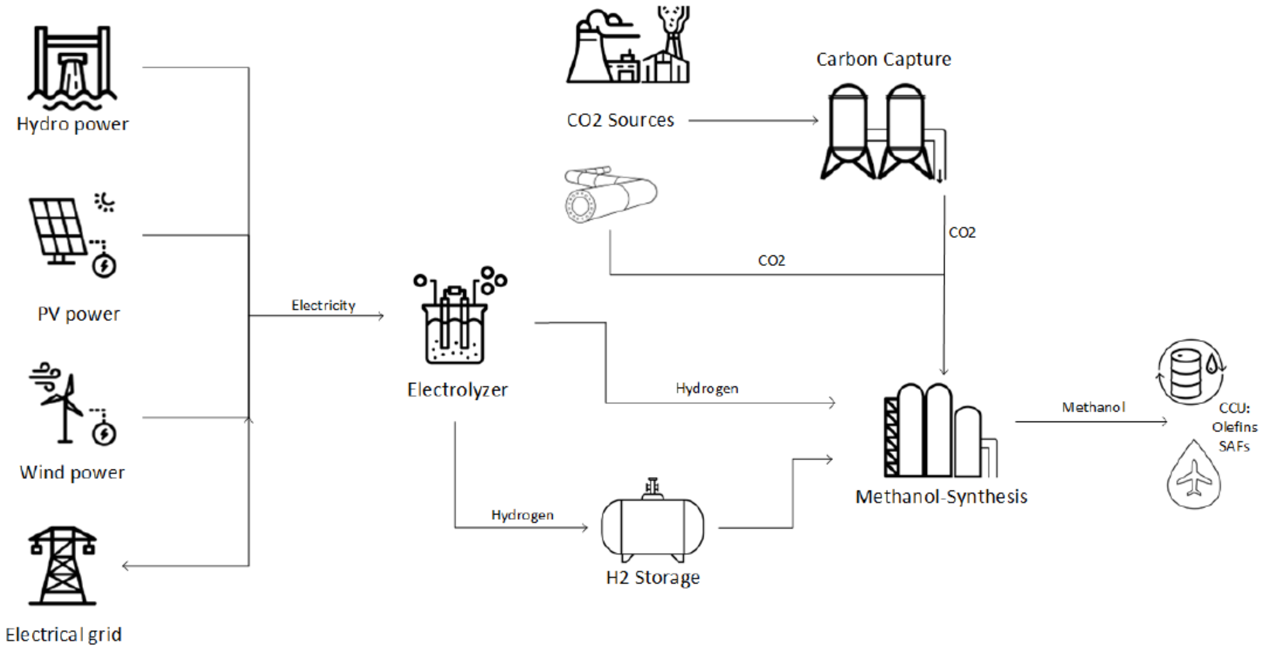
Schematics of a plant for the production of carbon-neutral fuels and chemicals



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SYNTHETIC CARBON NEUTRAL CHEMICALS

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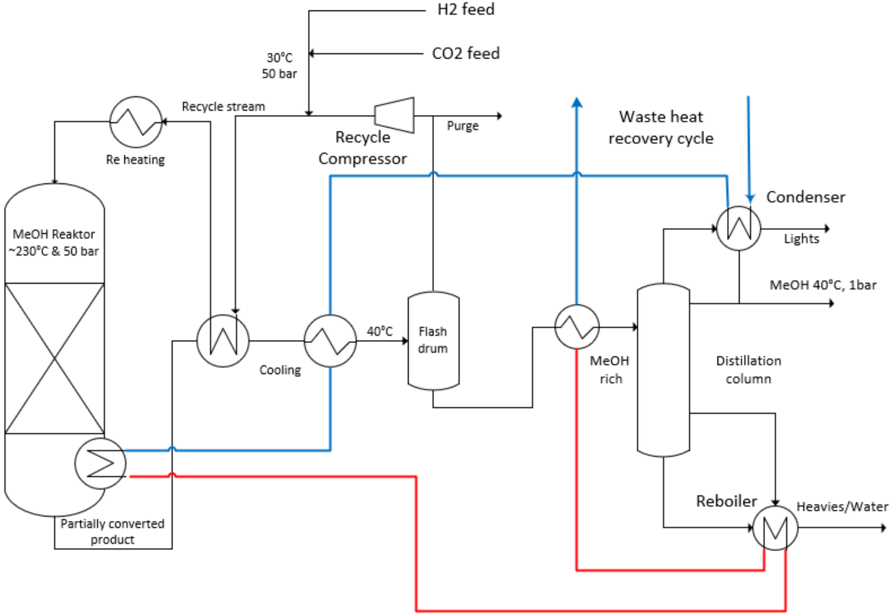
"Green methanol" as a "platform chemical"

Schematics of "green methanol" synthesis



- Methanol is synthesized from **"green hydrogen" and "biogenic CO2"** via…
- …**"CO2 hydrogenation"** in a cooled reactor followed by distillation (utilizing waste heat from the MeOH-reactor)
- Methanol is one of the required **bulk chemicals**
- Methanol will be used as future **ship fuel**

SYNTHETIC CARBON NEUTRAL CHEMICALS

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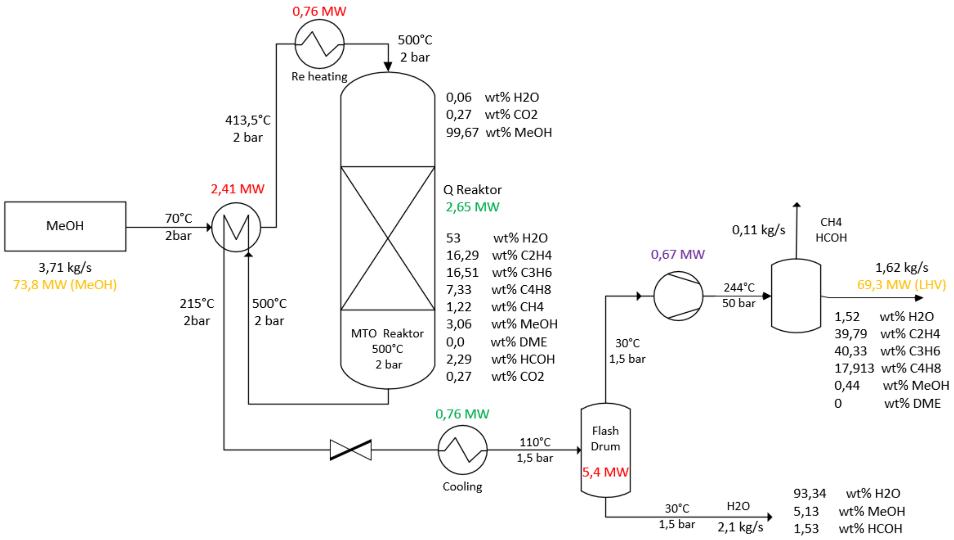
"Green methanol" as a "platform chemical"

Example of "Methanol-to-Olefin" synthesis



- **Light Olefins** are produced **via "Methanol-to-Olefin"** process (MTO)
- Products include **ethylene, propylene, butylene, formaldehyde, DME**
- The exact product **mixture depends on catalyst, reactor details and process conditions**
- The **MTO-process** is rather mature and **available on an industrial scale**

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SYNTHETIC CARBON NEUTRAL CHEMICALS

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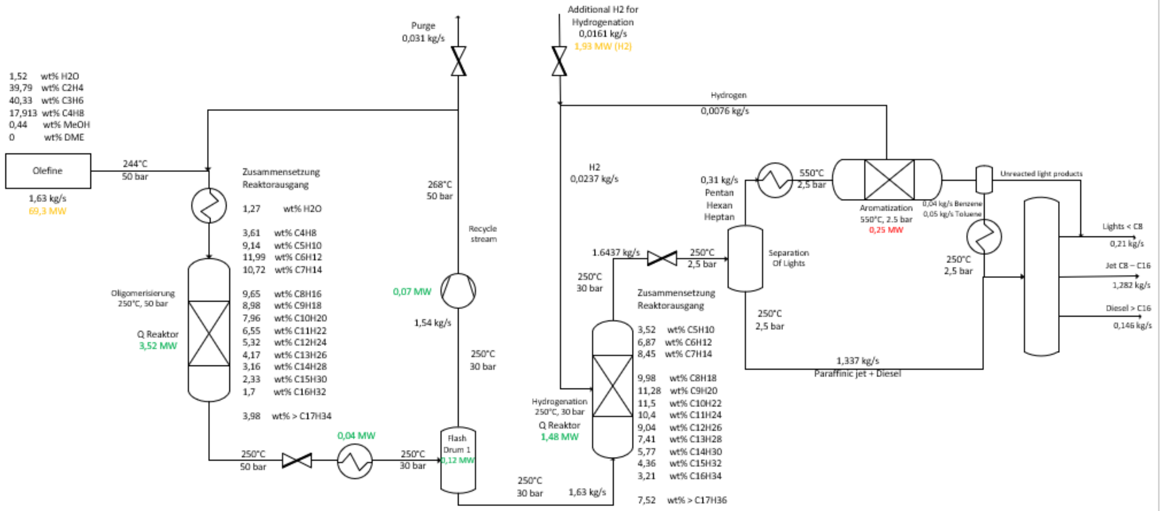
“Green methanol” as a “platform chemical”

Example of “Olefin-to-Jet/BTEX” synthesis



- **e-SAF and BTEX** are produced via a combination of MTO and MTA combined with oligomerization, hydrogenation and distillation
- A **variety of “green chemicals and fuels” can be synthesized** according to future market demand.
- The process principles are well understood, **upscaling and optimization is ongoing**.

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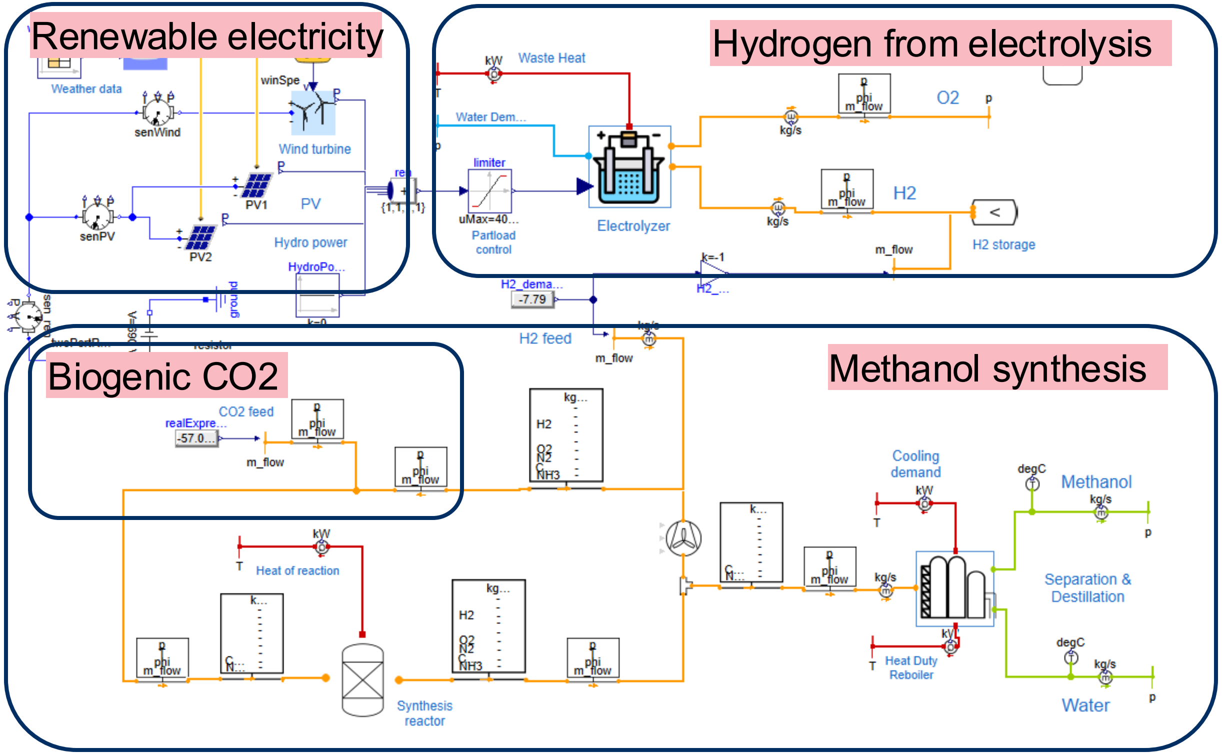
PROCESS MODELLING

Design, modelling and simulation of the production of “green methanol”

AIT employs Dymola/Modelica to physically model the whole process

- **Green electricity** from renewables
- Production, transport and storage of **hydrogen**
- Capture, transport and storage of **biogenic CO2**
- **Synthesis processes** of green chemicals and fuels



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MODELLING OF RENEWABLES

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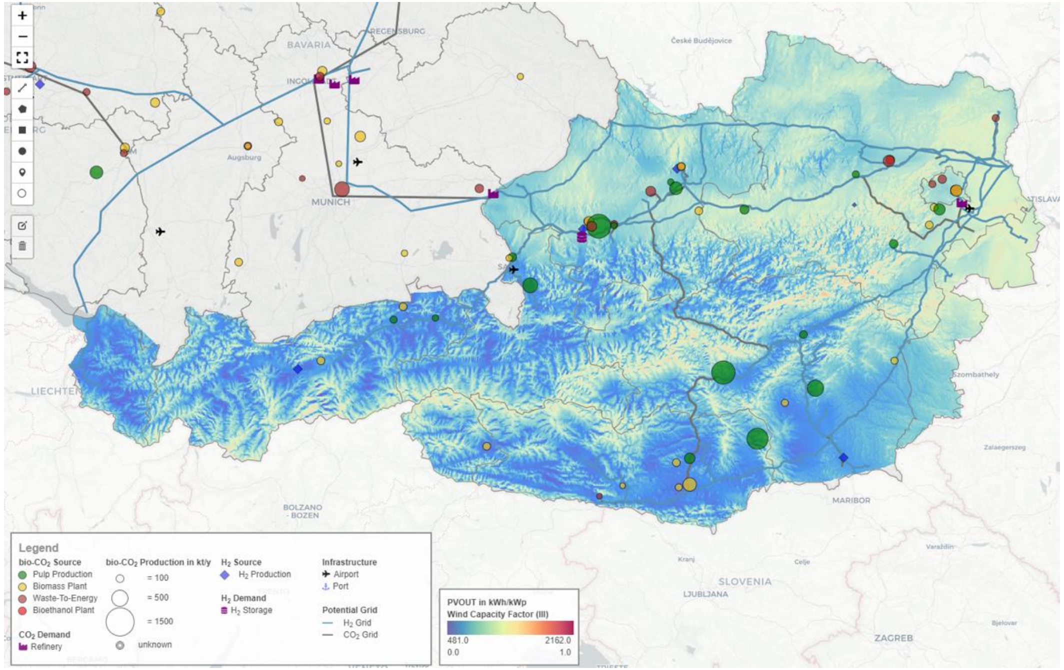
Design, modelling and simulation of the production of "green methanol"

- Real GIS-based **weather data** is used for all **renewables**
- **AIT has developed a data base for all large biogenic CO2 sources** for many European countries and some selected international countries

The amount of "reasonably available carbon-neutral CO2" is setting the limit for the amount of green chemicals and fuels that can be produced.



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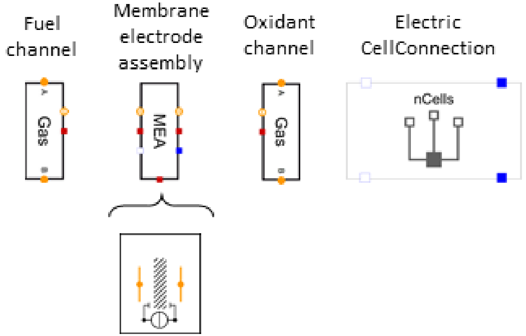
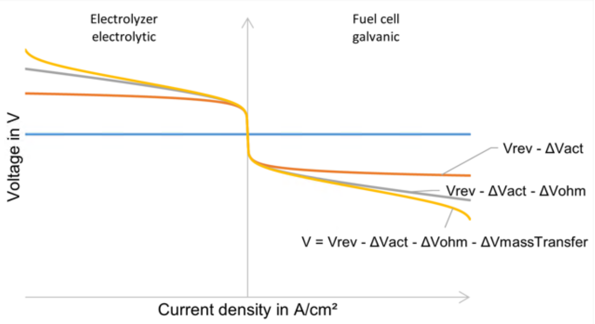
MODELLING OF H2 AND SYNTHESIS

Electrolyzer model





All plant components are modelled in their relevant physical domains:

- electrical
- thermal
- chemical

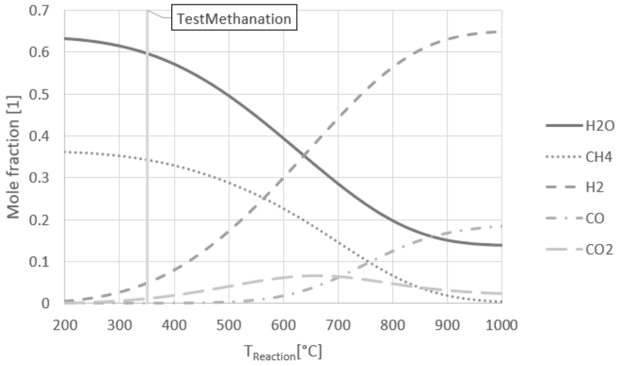
Models for chemical reactors

SMR "CH4 + H2O <-> 3H2 + CO",

WGSR "CO + H2O <-> H2 + CO2");

$$r = \frac{1}{\nu_A} \cdot \frac{d[A]}{dt} = k \cdot [A]$$

$$r_{SMR} = x_{CH4} \cdot x_{H2O} \cdot p \cdot 4274 \cdot 10^{-5} e^{-\frac{82000}{R \cdot T_{wall}}}$$



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SIMULATION

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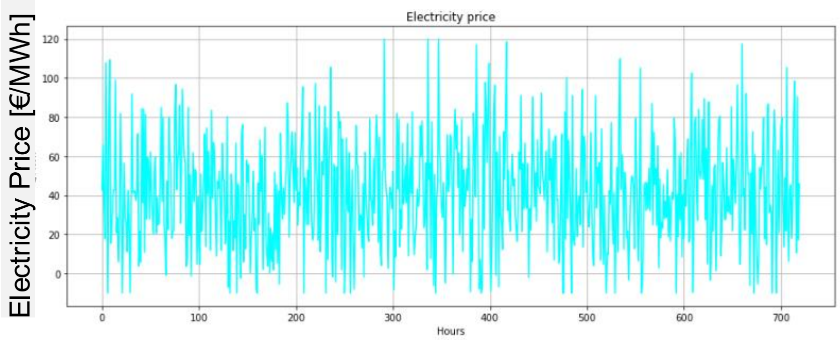
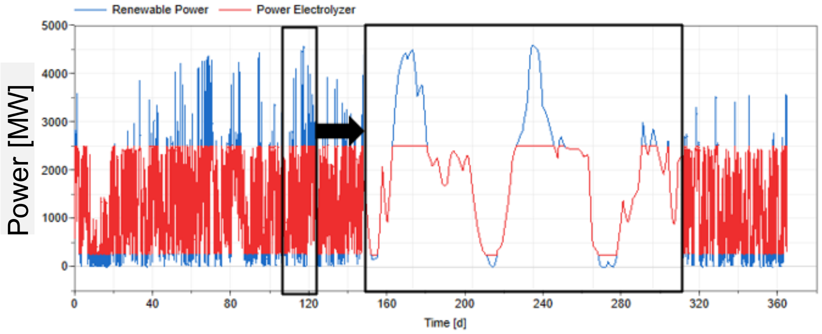
Annual simulation with seconds time resolution are performed





- **Markets** for electricity and green chemicals and fuels are implemented
- Different **control strategies** are developed and compared
- **Sizing of all plant components** is performed via optimization

SIMULATION RESULTS

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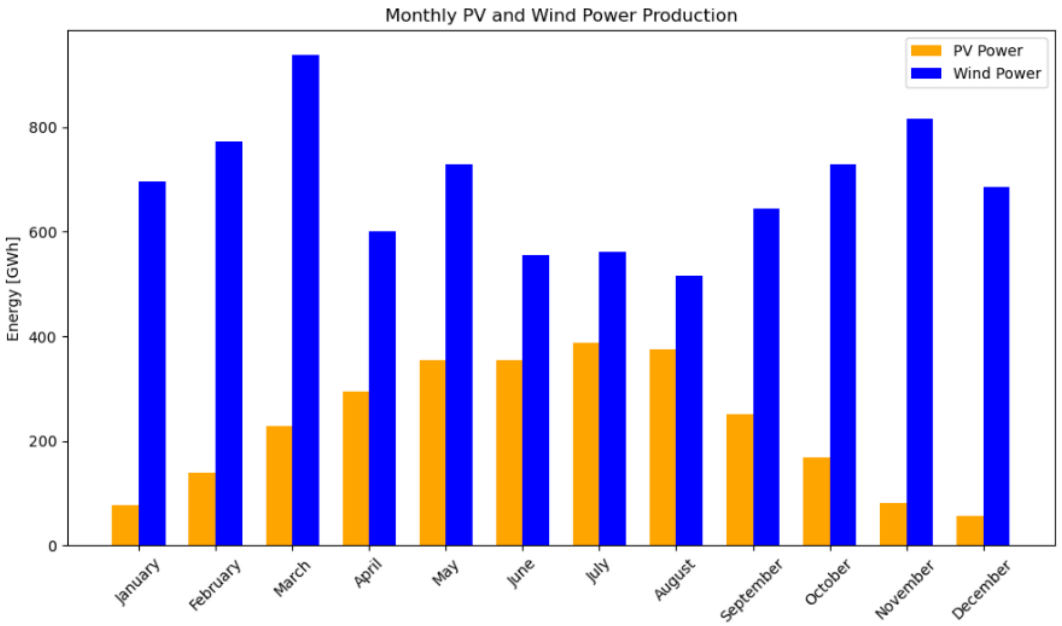
Example: Production of 1.3 Mt/year of "green methanol" in Austria

- Due to the RNFBO regulations, **additional renewables** have to be installed
- Additional Austrian hydro potential is limited
- **Hybrid wind and PV parks** provide the optimal annual production profile
- **Optimal size of renewables**:
  - Wind power: 2.44 GW
  - PV power: 2.19 GW



SIMULATION RESULTS

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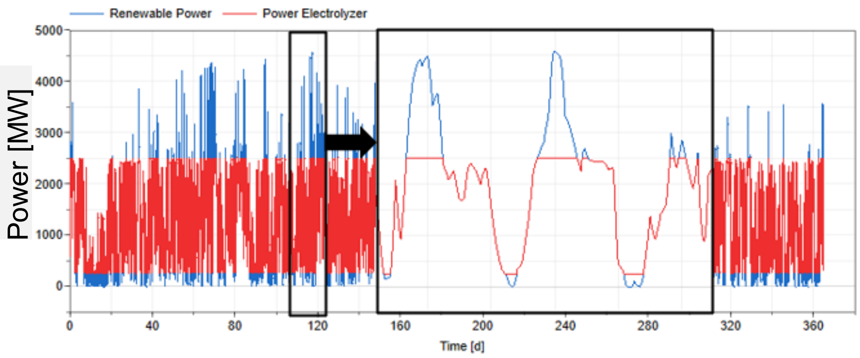
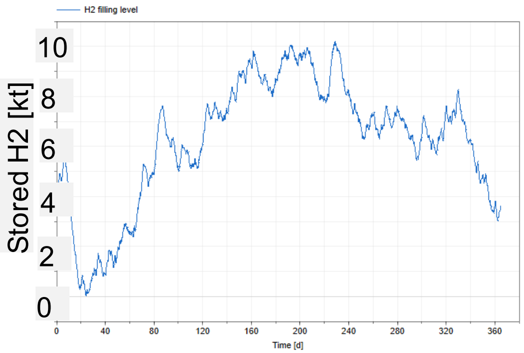
Example: Production of 1.3 Mt/year of “green methanol” in Austria

- **Synthesis reactors** prefer rather constant operation and thus “smooth” H2-input
- **Renewables are fluctuating →**
  - **Flexible electrolyzer** technologies are employed in combination with
  - Suitable **H2 storages**
- **Optimal size of H2-system**:
  - Electrolyzer power: 2.5 GW
  - H2 storage: 10 kt





SIMULATION RESULTS

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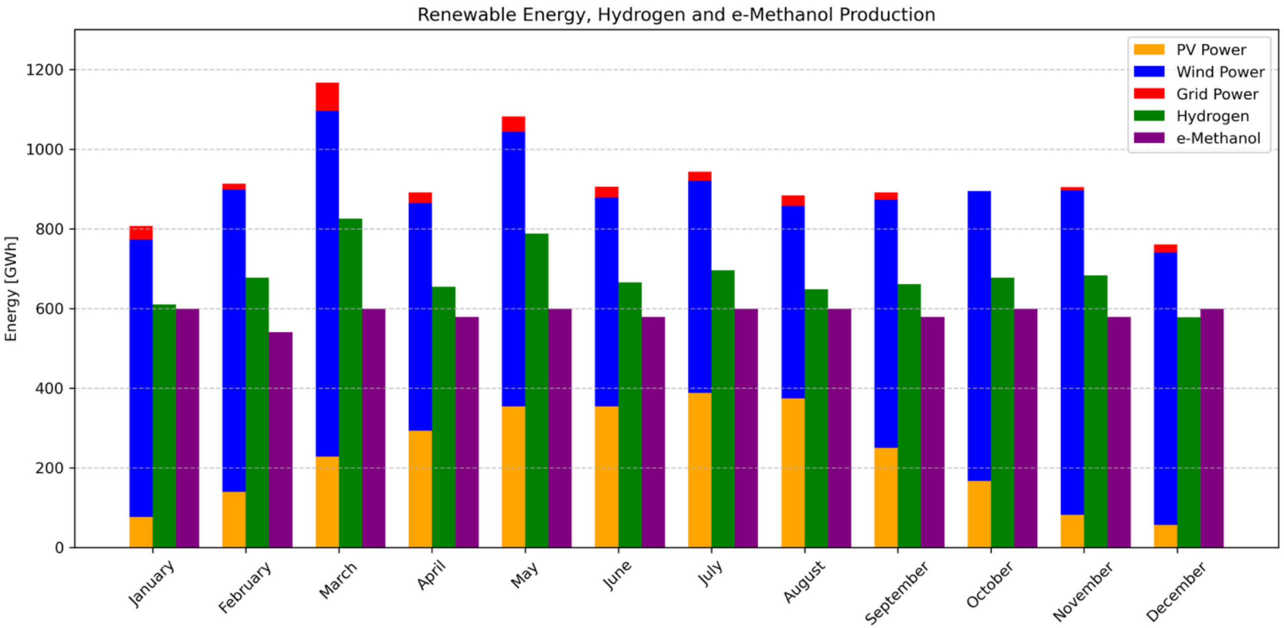
Example: Production of 1.3 Mt/year of "green methanol" in Austria

Methanol production	1.27	Mt/a
CO2 demand	1.78	Mt/a
Hydrogen production	243.5	kt/a



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SIMULATION RESULTS

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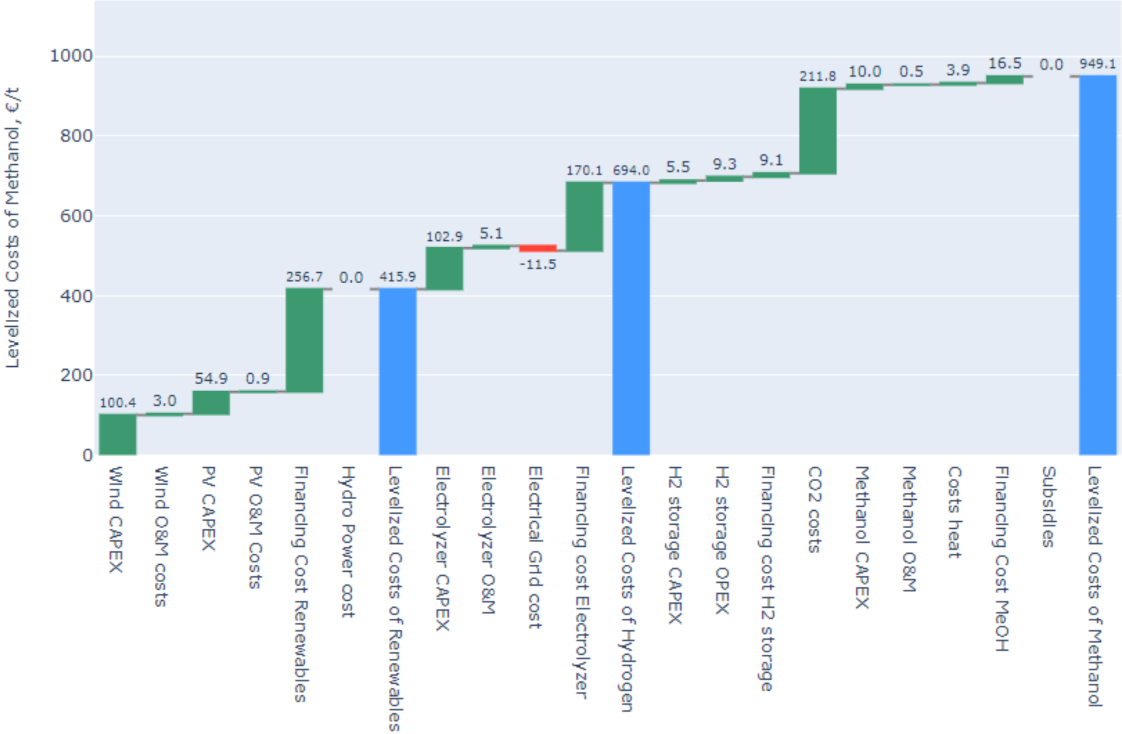
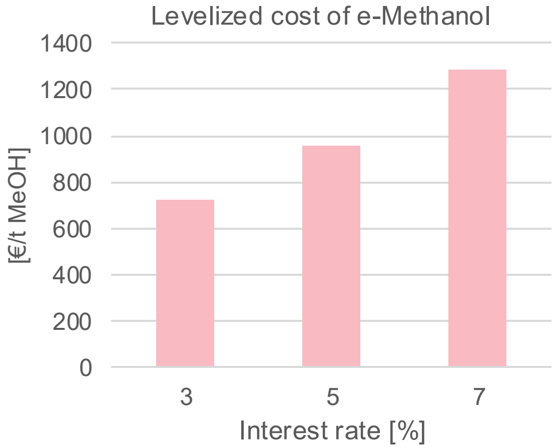
Example: production of 1.3 Mt/year of “green methanol” in Austria





The production costs of “green hydrogen” is the main cost driver for the production of green chemicals and fuels.

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Production of “green chemicals and fuels” in Austria in 2050

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SCENARIO DEFINITION

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Possible Austrian production of “green chemicals and fuels” in 2050

Scenario assumptions:

- **50% of the 2019 production volume of Olefins** will be produced in 2050 via the synthetic route, the other 50% via other routes or import
- **50% of the EU-quota for the synthetic fraction of SAFs** will be produced in Austria in 2050, the other 50% will be imported
- **100% of “higher hydrocarbons”, urea and BTEX** will be produced in Austria in 2050 via the synthetic route

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SIMULATION RESULTS

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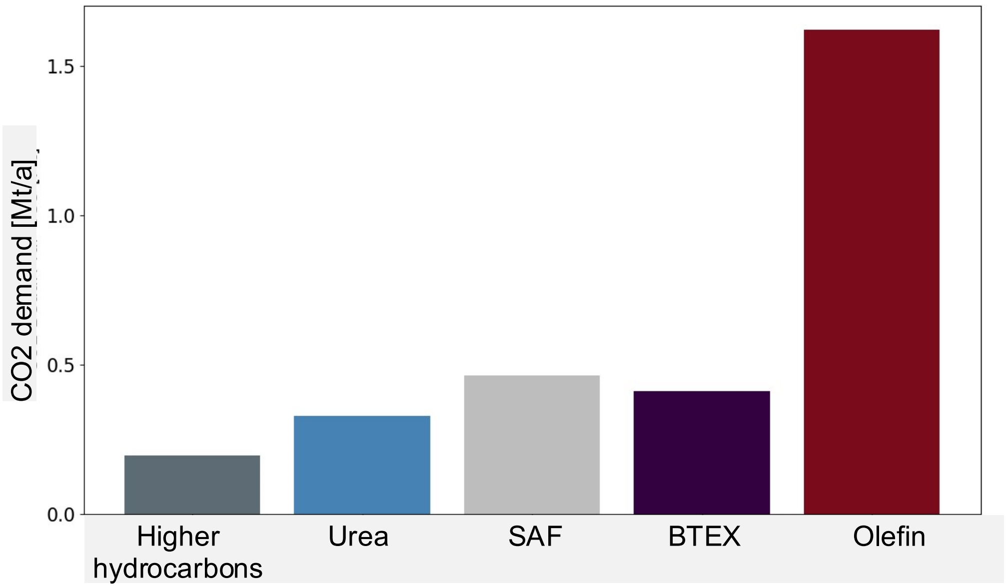
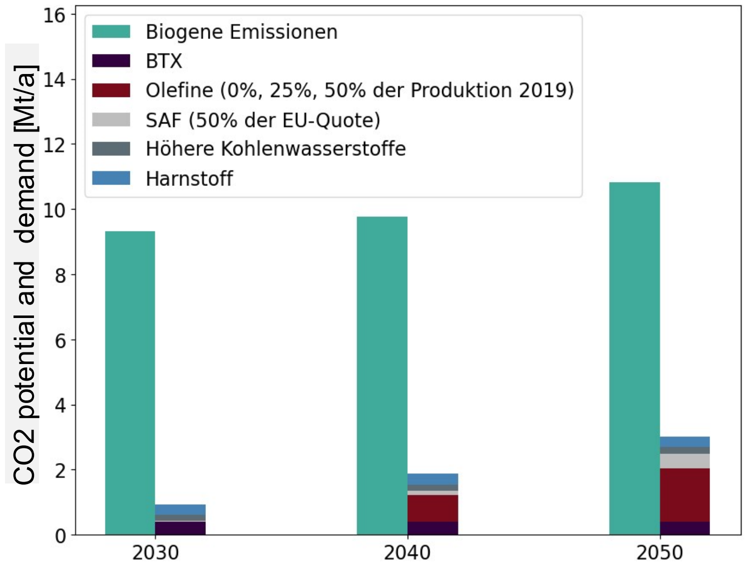
Possible Austrian production of "green chemicals and fuels" in 2050

Demand of biogenic CO2



Availability of biogenic CO2



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SIMULATION RESULTS

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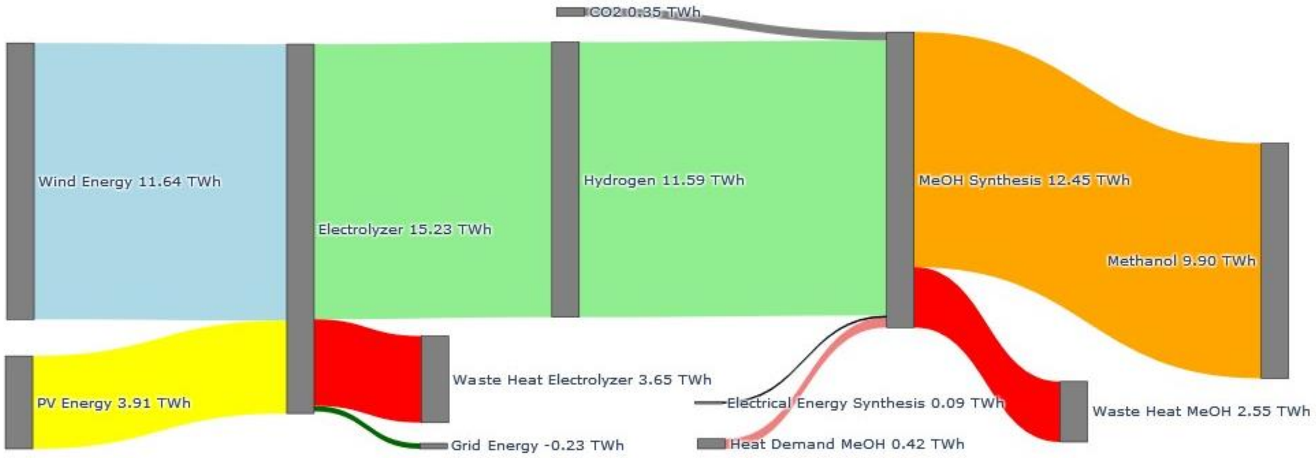
Possible Austrian production of “green chemicals and fuels” in 2050

Technical KPIs

Wind Power	3.5	GW
PV Power	3.1	GW
Renewable electricity production	16	TWh
Green H2 production	350	kt/a
Biogenic CO2 demand	2.6	Mt/a
Methanol production	1.8	Mt/a

Energy flow diagram



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SUMMARY

- International and European regulations demand quota for „green fuels and chemicals“

- This leads to huge markets at a scale of 100 Mt/a production volume

- Biogenic, recycle and synthetic routes are necessary to fulfil the requirement

- Synthetic fuels and chemicals are produced from “green hydrogen” and “biogenic CO2”

The Austrian potential for the production of economically viable “green chemicals and fuels” is very good due to competitive renewables and an excellent potential of biogenic CO2

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THANK YOU FOR YOUR ATTENTION!

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