Optimal design of synthetic methane production sites incorporating direct air capture technology

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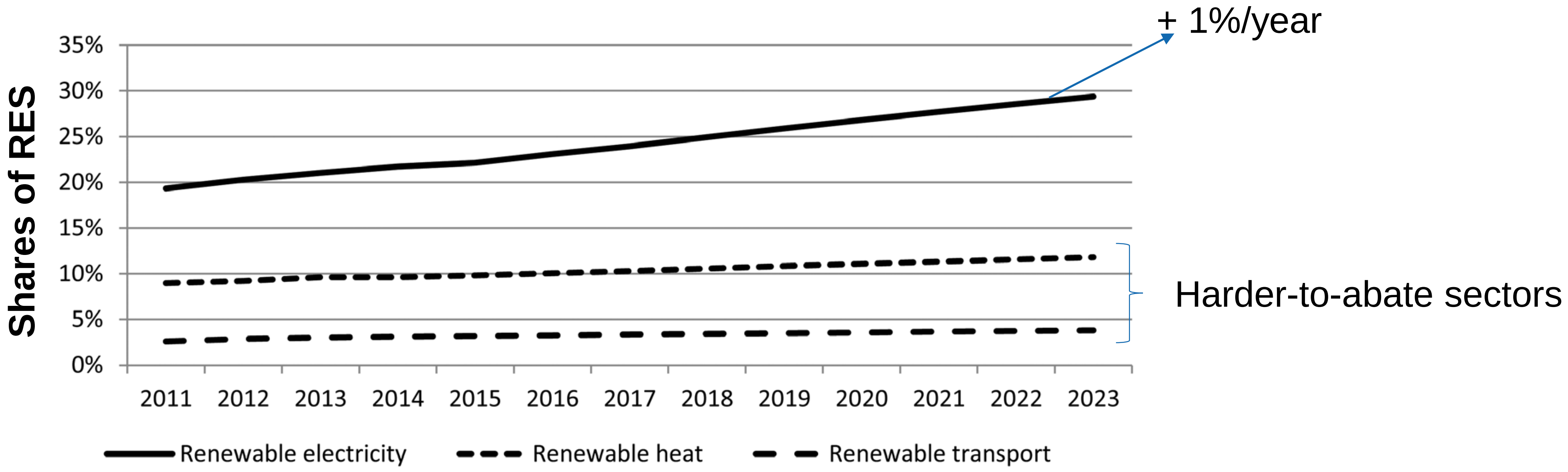
On the way to Decarbonization – electrification

- Globally, renewable energy source (RES) has tripled from 1990 to 2020, accounting for 12.5% of the global primary energy supply;
- RES technologies are primarily available in the **power sector**, making **electrification** a key strategy for decarbonisation.

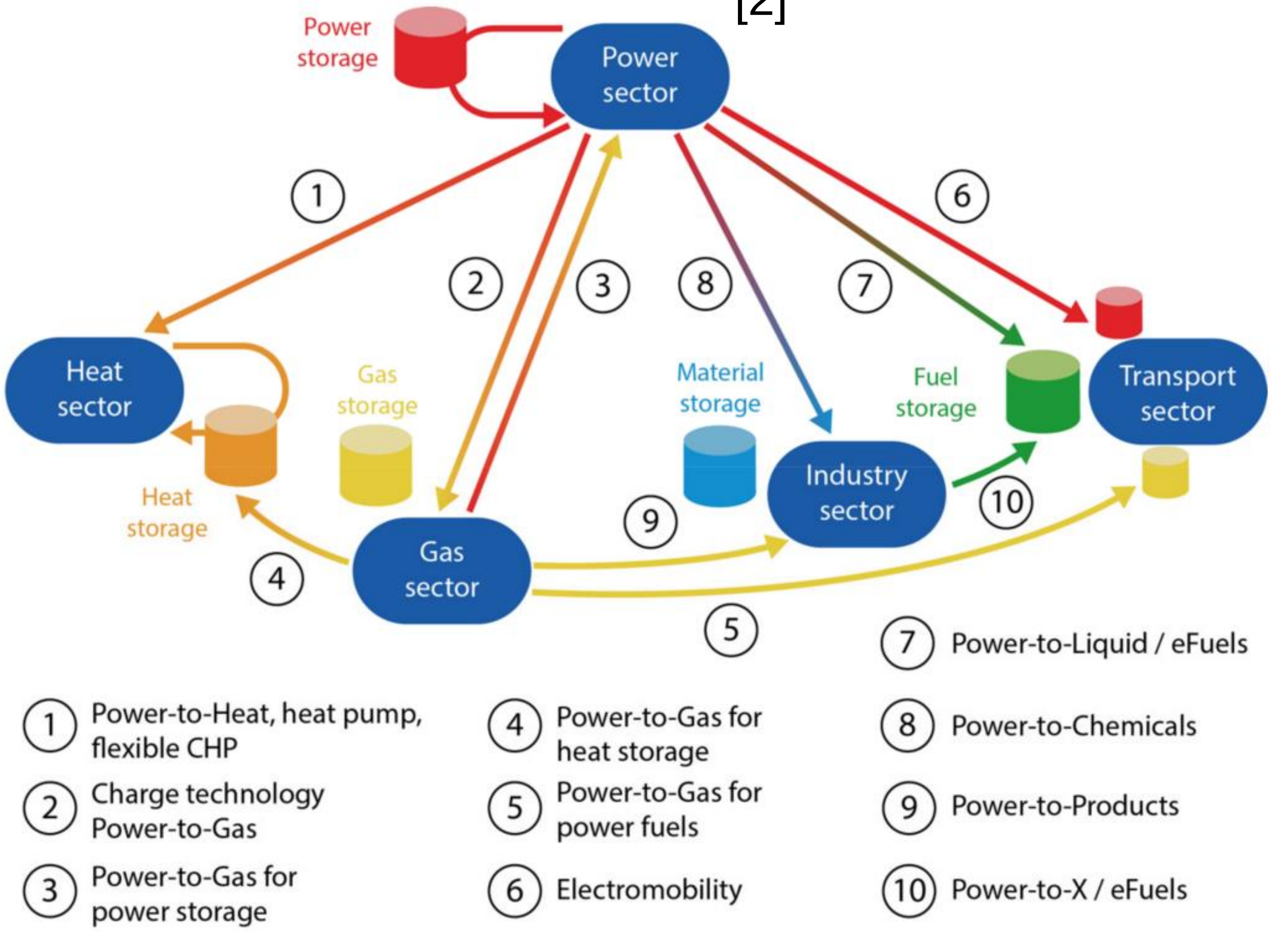


Philbert C., Direct and indirect electrification of industry and beyond, 2019

Harder-to-abate sectors

- Direct electrification is challenging in certain sectors (**“harder-to-abate” sectors**), such as aviation, shipping, heavy-duty road transport, etc. [1];
- **Power-to-X (PtX)** is one of the ways to achieve full decarbonisation;
- PtX is a collective term for conversion technologies that **turn electricity into carbon-neutral synthetic fuels**, such as hydrogen, synthetic natural gas, liquid fuels, or chemicals.

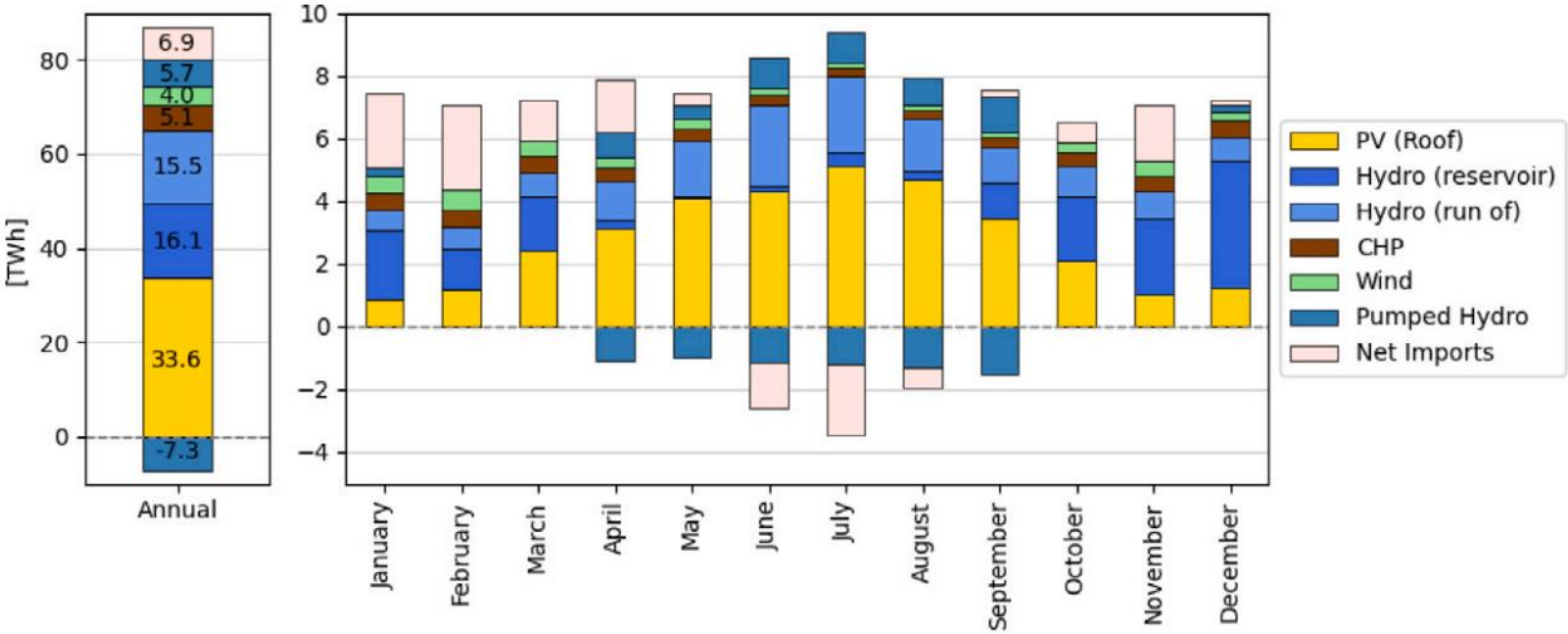
[2]



[1] Philbert C., Direct and indirect electrification of industry and beyond, 2019
[2] Sterner et al., Power-to-Gas and Power-to-X—The History and Results of Developing a New Storage Concept, 2021

The winter problem

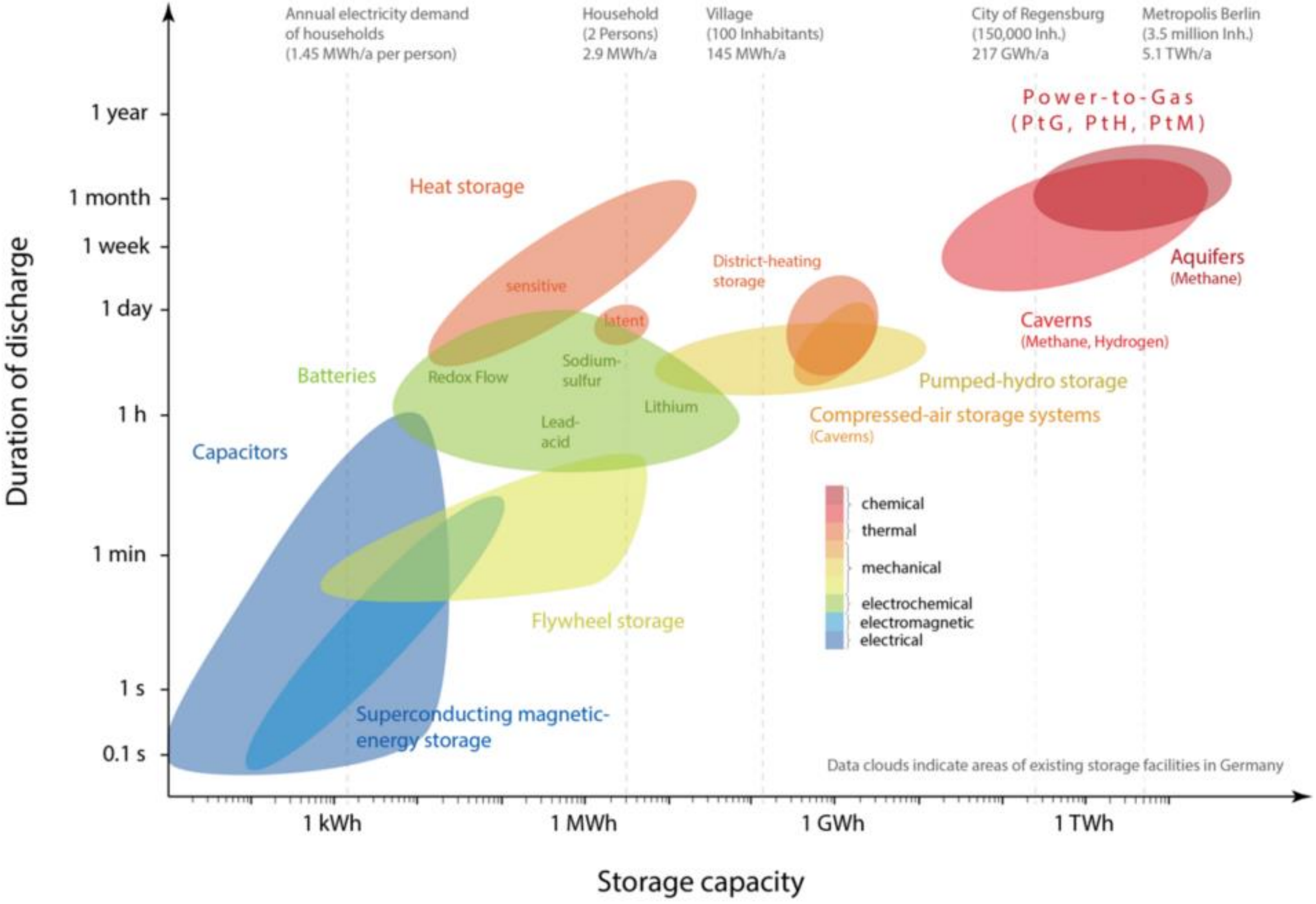
- RES generation is characterized by **intermittency** and **seasonality**;
- In the instance of Switzerland, electricity is exported in summer (excess) and imported in winter (deficit) to/from neighbouring countries.



Mellot et al., Mitigating future winter electricity deficits: A case study from Switzerland

PtX for long-term storage

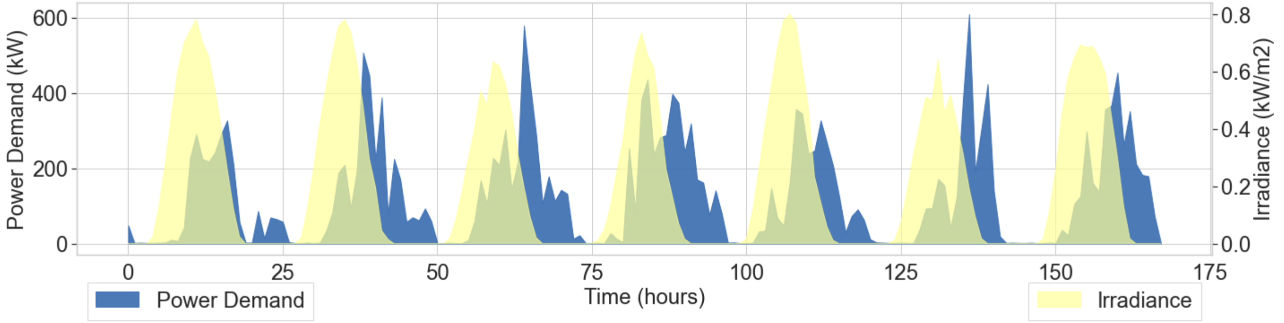
- How to face intermittency and seasonality?
- Storage solutions are and will be key components of energy systems;
- **Chemical storage** is a promising way to store large amount of energy for long times;

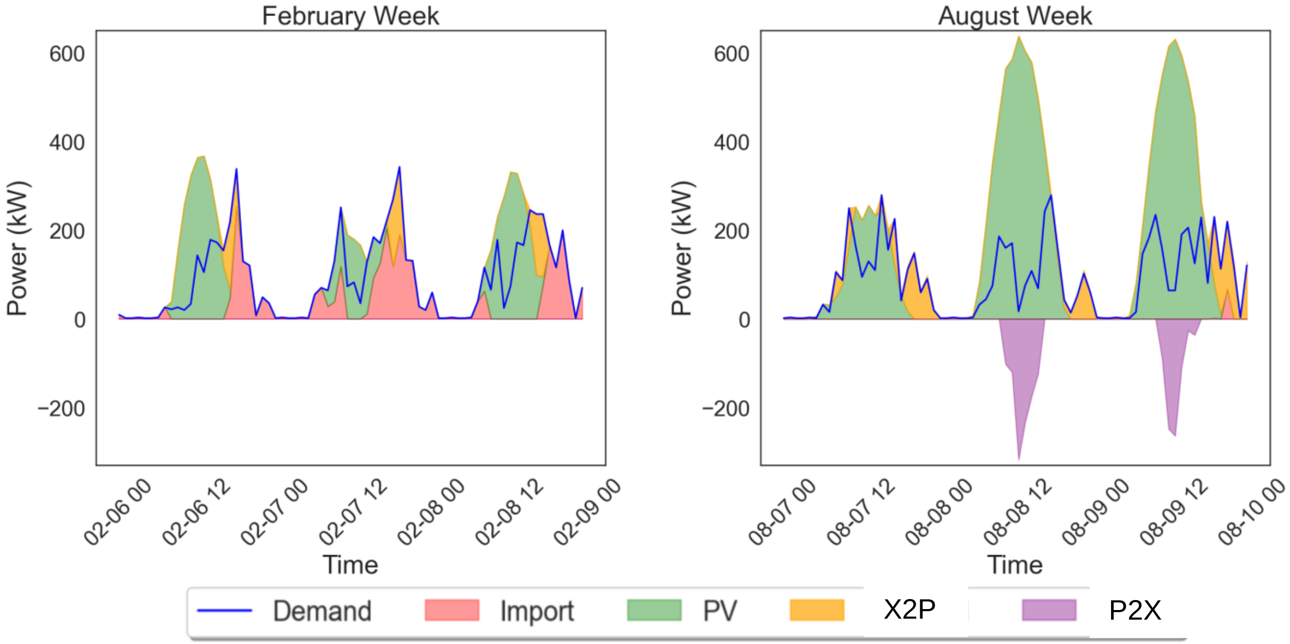


[1] Sterner, M.; Stadler, I. Handbook of Energy Storage: Demand, Technologies, Integration; Springer: Berlin/Heidelberg, Germany, 2018; ISBN 978-3-662-55503-3.

Balance between supply and demand

- Power-to-X can also be used in the **short-term** to avoid grid congestion and balance energy supply and demand;
- Sudden excess of electricity production can be converted into fuel;
- Reserve of fuel, e.g. hydrogen, can be used to cover unexpected increases of energy demand or to avoid peaks;





Figures from Maxime Fischer

Swiss Energy system in 2050

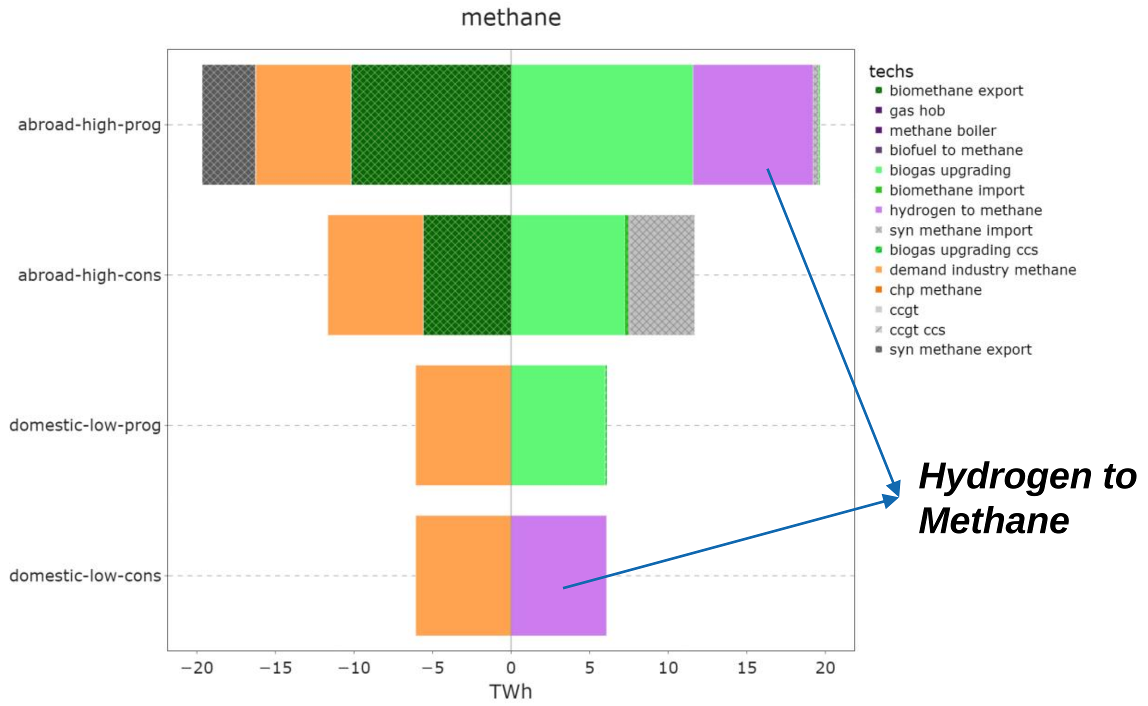


Figure 3.15: Yearly balance of methane fuel production and consumption in Switzerland in all four scenarios.

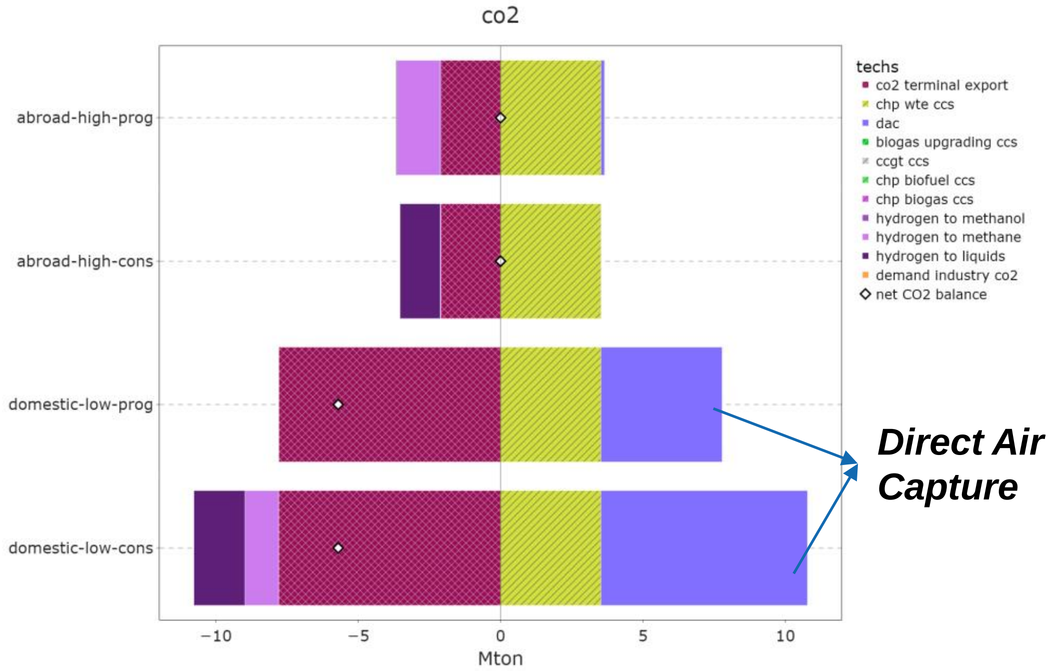
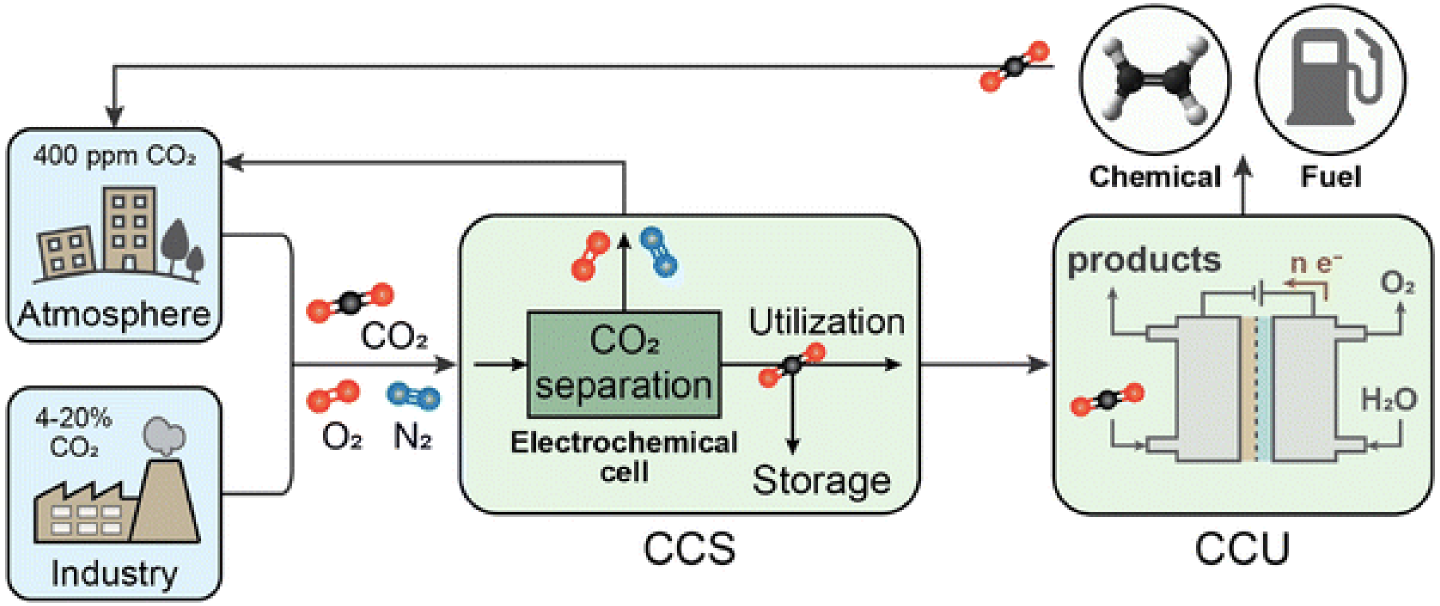


Figure 3.18: Yearly balance of captured CO_2 sources and uses in Switzerland in all four scenarios. The marker shows the national net carbon balance. The category CO_2 terminal export represents permanent sequestration of the CO_2 abroad.

Sanvito, F., Garrison, J. (2024). The role of flexibility and sector coupling in the Swiss energy system. SWEET PATHFNDR

Summary of motivations for PtX technologies

1. Renewable energy sources are intermittent and seasonal → **long-term storage solution**
2. Effective way to balance supply and demand → **flexibility provision**
3. Provide a way to decarbonize harder-to-abate sectors → **sector coupling**
4. Depending on the process, they might require CO_2 → **carbon capture and utilization**



Rahimi, M., A. Khurram, T.A. Hatton & B. Gallant , *Chem. Soc. Rev.* 51, 8676 (2022).

Key challenges for Power-to-X

1. **Complex systems to design**, build and operate;
2. Mainly for gas, challenges during storage periods;
3. **High costs for production**, transportation, distribution and use;
4. Low technology readiness levels**;**
5. **They require significant power for the operation;**

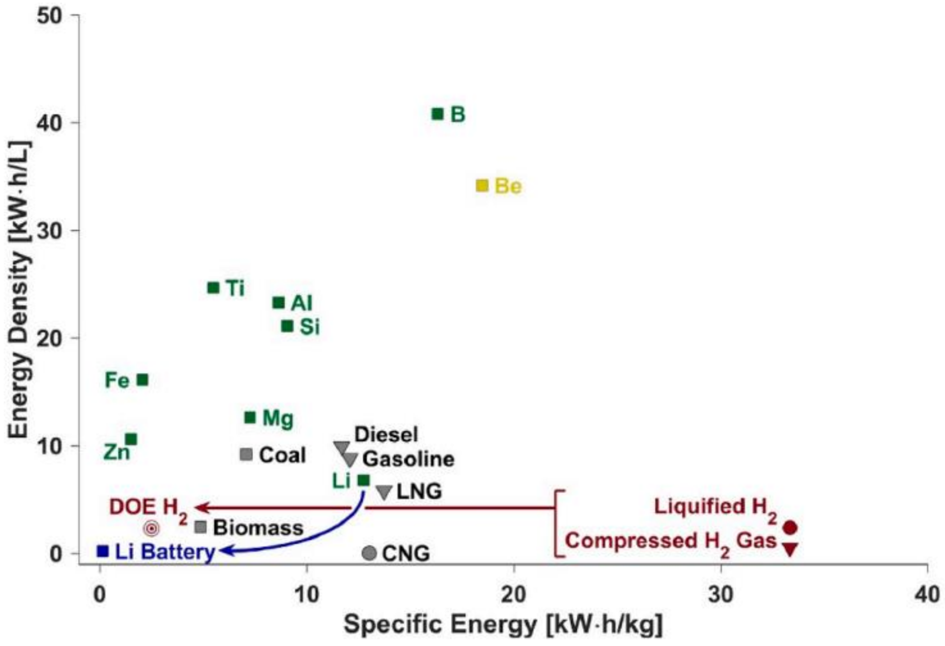


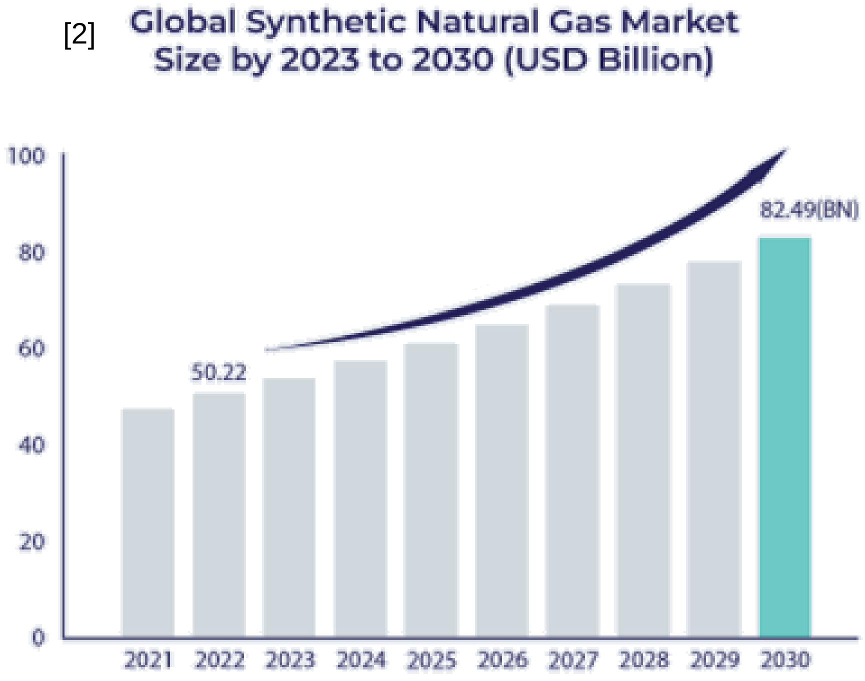
Fig. 4. Comparison between the volumetric energy density and specific energy with different types of energy sources, the data presented here does not take into account the storage tank system [17].

Ababneh et al., Electrofuels as emerging new green alternative fuel: A review of recent literature, 2022

Why Synthetic Methane?

- Compared to other synthetic fuels, synthetic CH_4 possesses a relatively high energy density and can rely on **existing infrastructures** [1];
- The production of synthetic CH_4 can utilize CO_2;
- The process to produce synthetic CH_4 is highly exothermic, thus providing good potential for optimal thermal management;

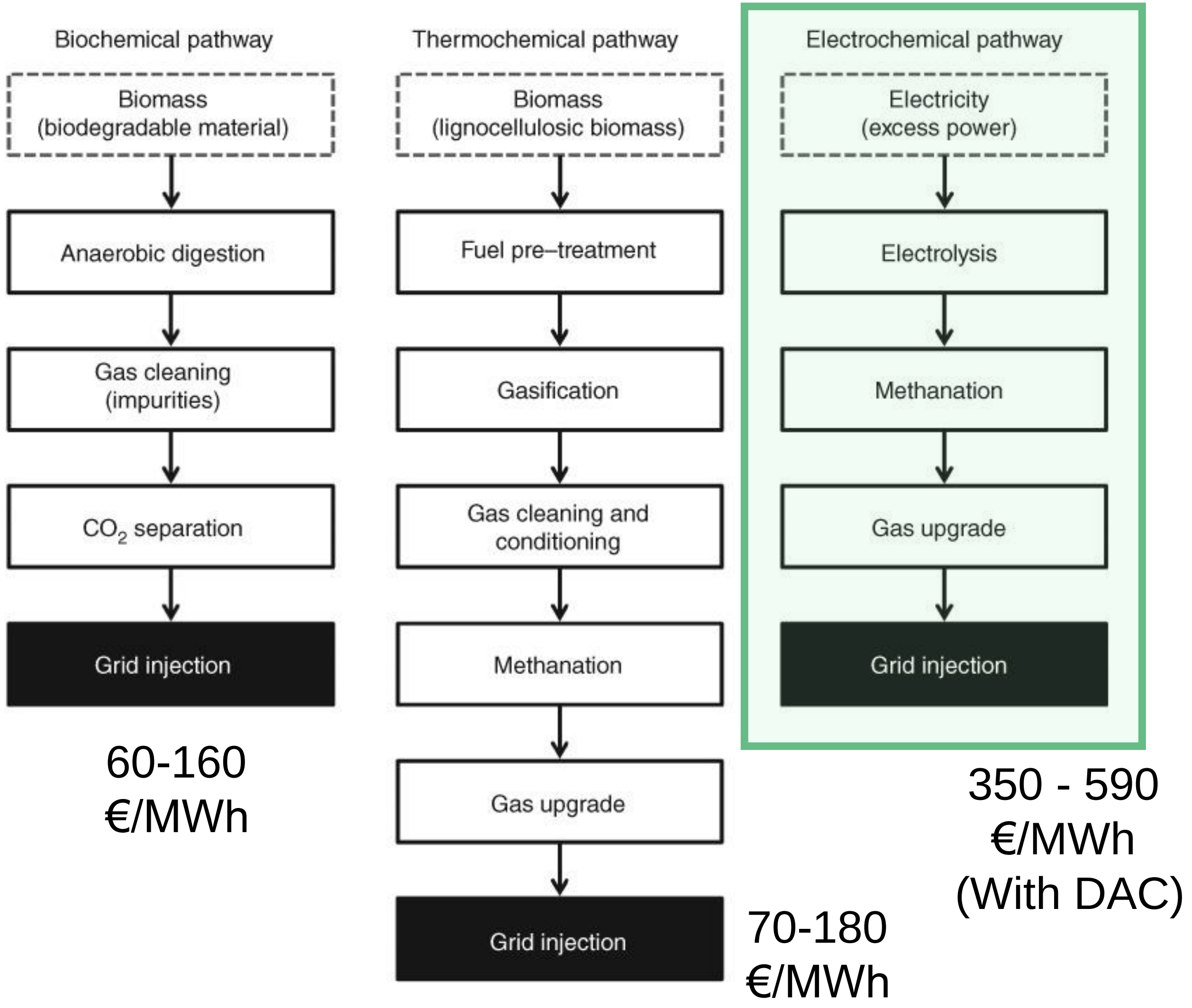
[2]



[1] Seyed Mojtaba Alirahmi et al., Renewable-integrated flexible production of energy and methane via re-using existing offshore oil and gas infrastructure, Journal of Cleaner Production, 2023
[2] SNS insiders, Synthetic Natural Gas Market, 2023

How is synthetic methane produced?

- There are several ways of producing synthetic methane;
- The electrochemical pathway does not require biomass and can exploit excess of electricity (RES);
- However, currently, **costs are too high**.
- Selling price of NG in Switzerland: 130 €/MWh to 170 €/MWh



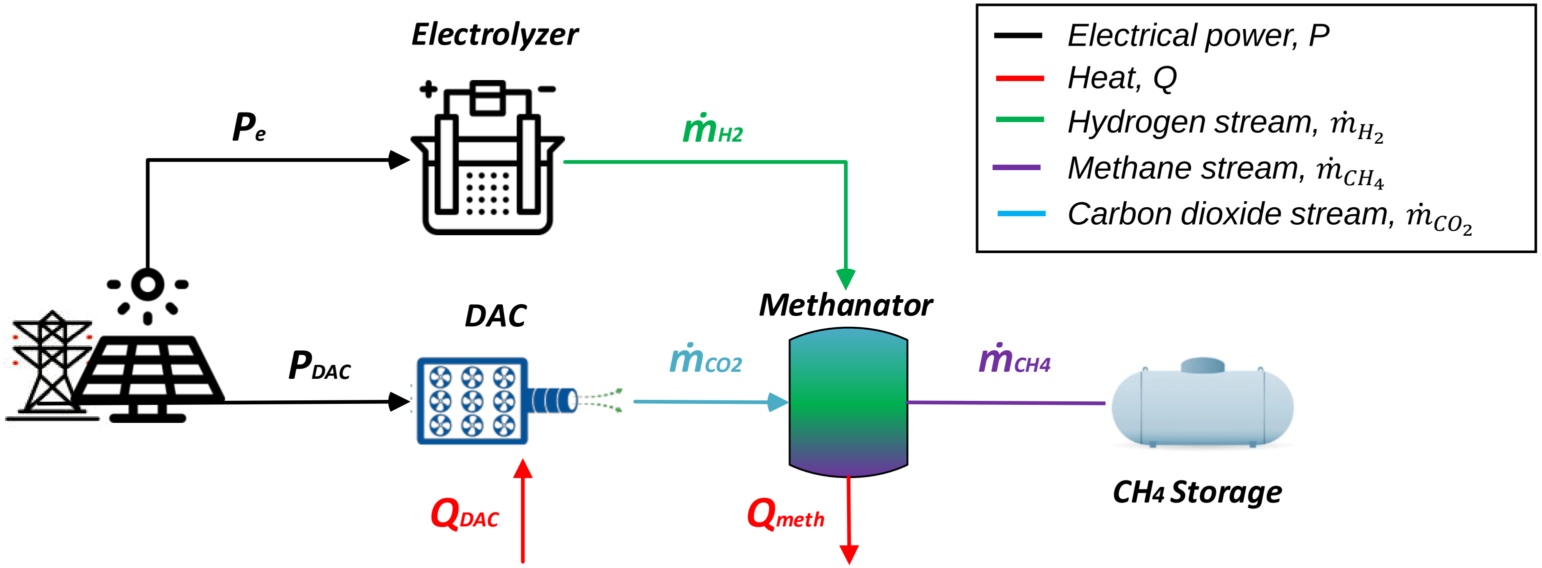
Fendt et al., Comparison of synthetic natural gas production pathways for the storage of renewable energy, 2015

Electrochemical pathway - Sabatier reaction

Among the different ways of producing synthetic methane, we focus on the Sabatier process:

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O + 164.9\ kJ/kg_{CO2}$$

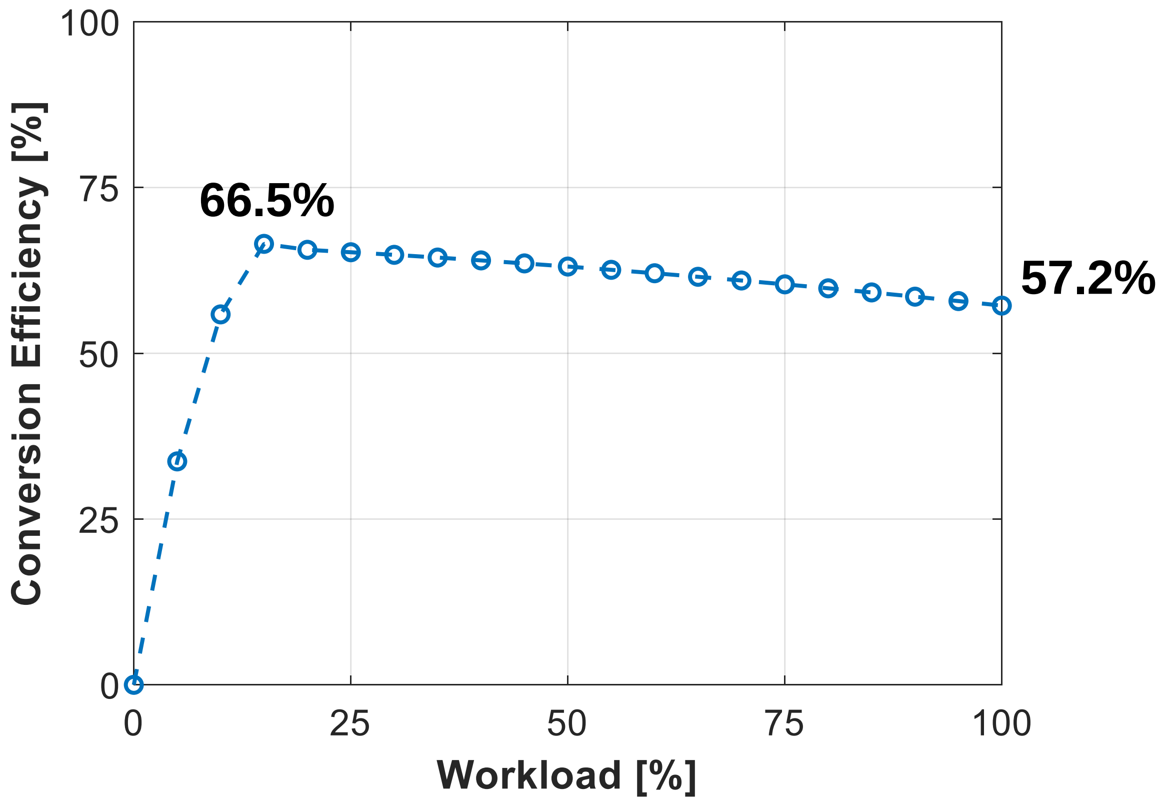
Key advantages: it utilizes CO_2 , it can be powered by RES and it is exothermic



Simplified schematic of a synthetic methane production site relying on the Sabitier process

Proton Exchange Membrane (PEM) electrolyzers – performance

- PEM electrolyzers uses electricity to split water into hydrogen and oxygen;
- PEM operates with high responsivity (ramping rates ≈2.5 to 8 $\%_{size}$/s) and produce H2 at high-quality;
- The production of 1 kg of H2 requires ≈58 kWh at nominal point and ≈50 kWh at the point of maximum efficiency;
- Energy consumption depends on how electrolyzer is operated and sized.

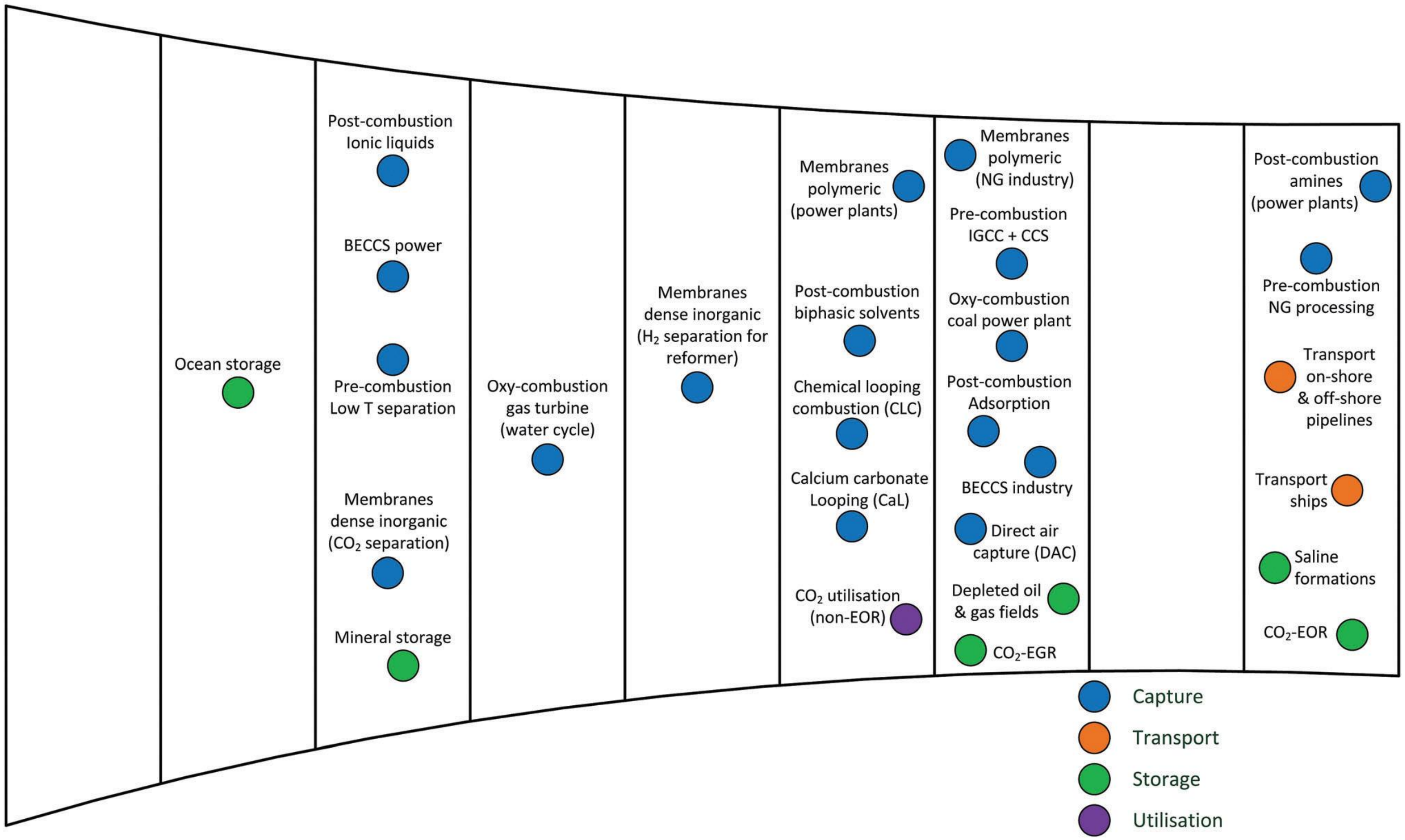


Conversion efficiency versus workload for a 180 kW electrolyzer at Empa.

Ways to capture CO_2

- CO2 can be removed from either the point source emission or directly from the air;
- Direct air capture (DAC) as the key advantages of **scalability** (large-scale deployment) and it does **not have geographical constraints.**

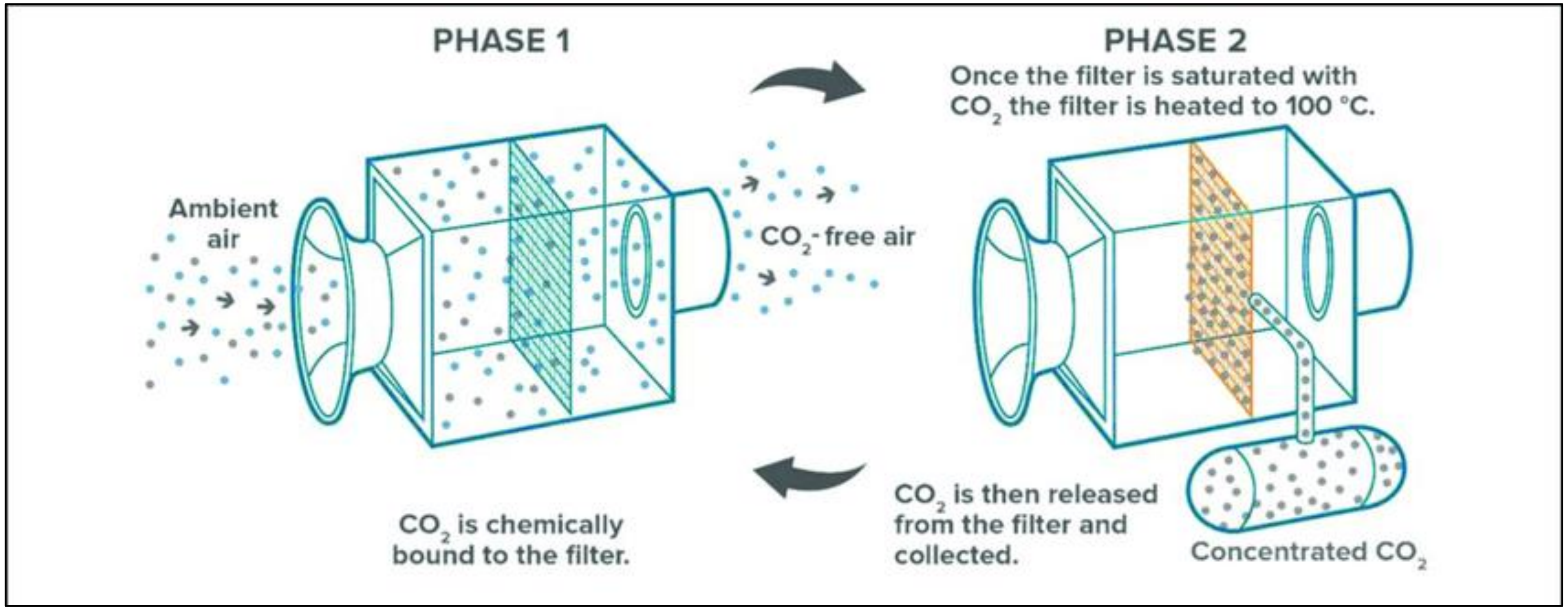
Concept	Formulation	Proof of concept (lab tests)	Lab prototype	Lab-scale plant	Pilot plant	Demonstration	Commercial Refinement required	Commercial
TRL1	TRL2	TRL3	TRL4	TRL5	TRL6	TRL7	TRL8	TRL9



Bui et al. 2018, Carbon capture and storage (CCS): the way forward

Direct Air Capture (DAC) units – physical principle

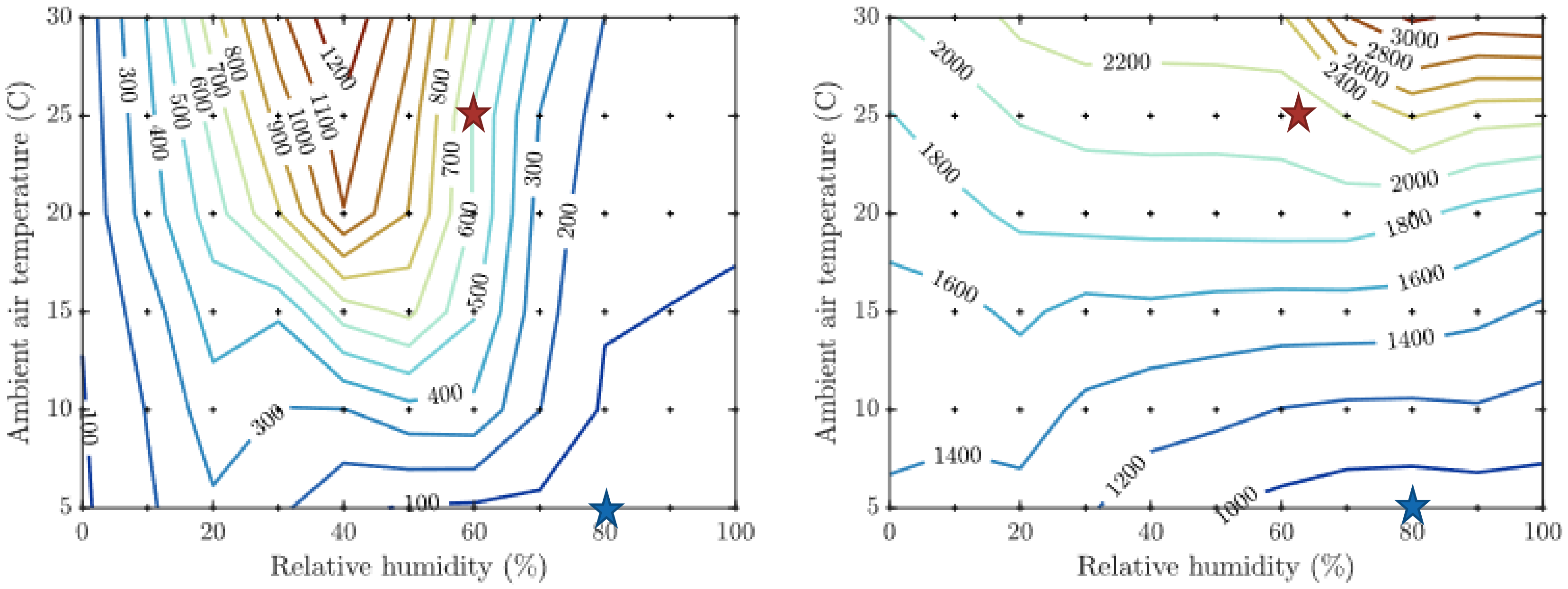
- DAC technologies can be situated independently of emission sources and can be powered by RES;
- Solid-sorbent DAC **requires both heat** (≈100 °C) and **electrical power**;



Beuttler C., The Role of Direct Air Capture in Mitigation of Anthropogenic Greenhouse Gas Emissions, 2019

Direct Air Capture (DAC) units – energy requirements

- The DAC energy demand strongly **depends on the ambient conditions** [1].
  - For 5 °C and relative humidity of 80% → <100 kWh_{el}/t_{CO2} and <1000 kWh_{th}/t_{CO2}
  - For 25 °C and and relative humidity of 60% → 600 kWh_{el}/t_{CO2} and 2200 kWh_{th}/t_{CO2}

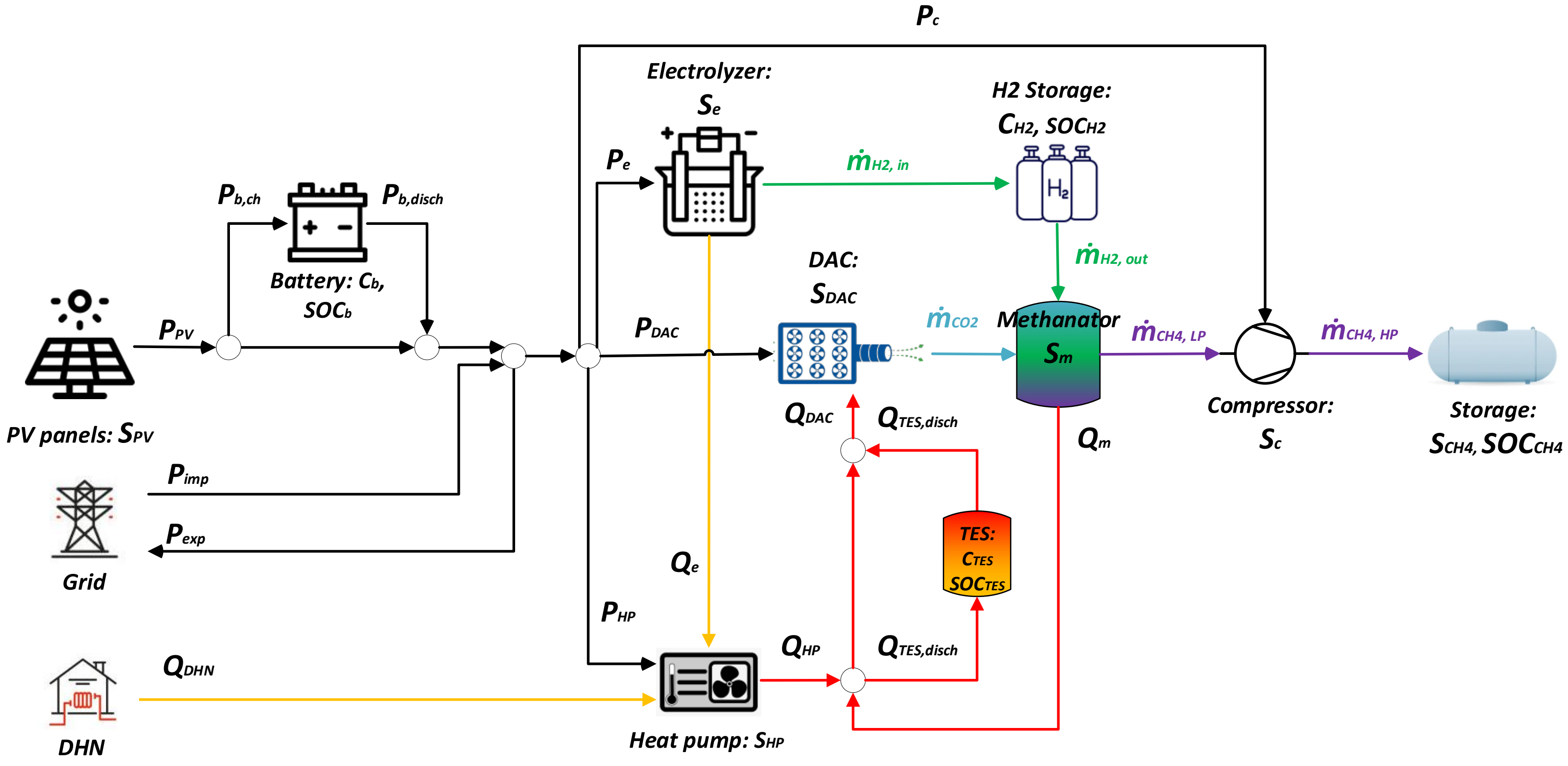


(a) Electric energy demand in kWh per t CO_2 captured

(b) Thermal energy demand in kWh per t CO_2 captured

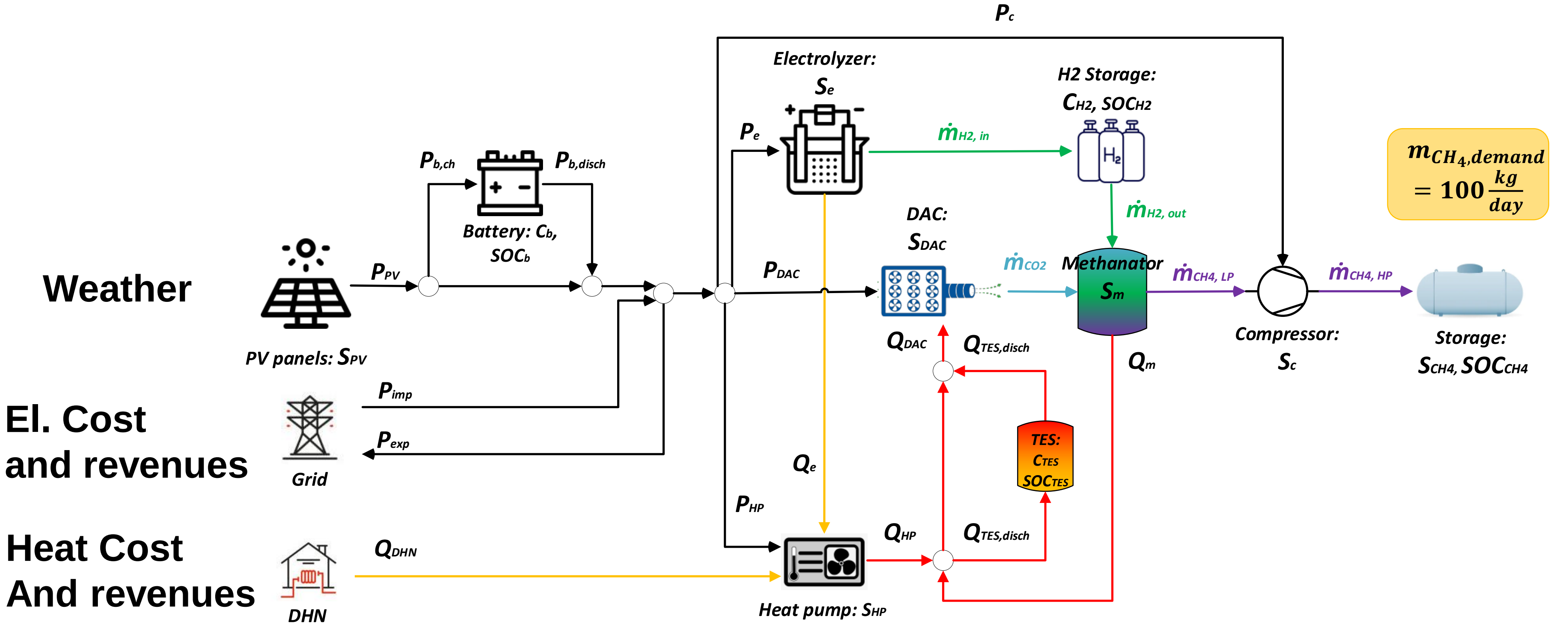
[1] *Wiegner et al., Optimal Design and Operation of Solid Sorbent Direct Air Capture Processes at Varying Ambient Conditions, 2022*

Optimal Design of Synthetic methane production sites



<u>Nomenclature</u>:
C: capacity [kWh]; S: nominal size [kW];
P: electrical power [kW]; Q: heat [kW];
SOC: State of Charge [-]; $\dot{m}$: mass flow rate [kg/s]

Optimal Desing of Synthetic methane production sites



$$m_{CH_4,demand} = 100\,\frac{kg}{day}$$

Production goal

<u>Nomenclature</u>:

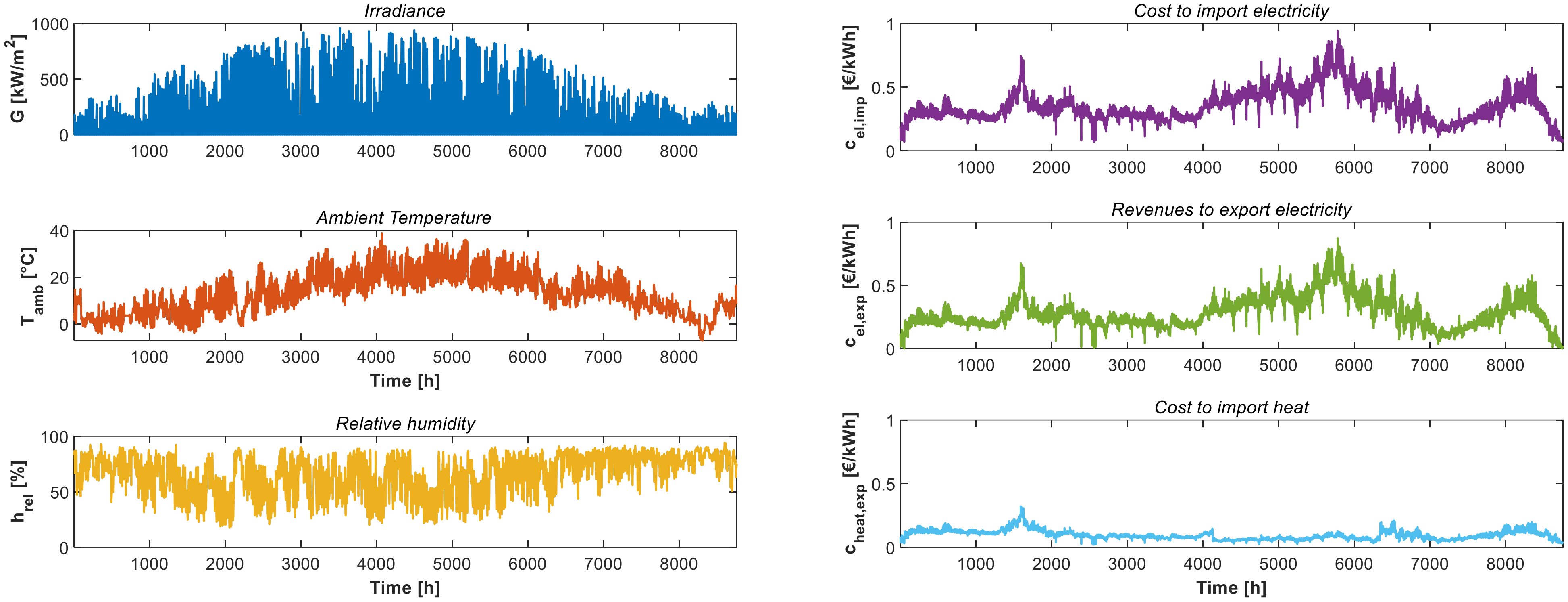
C: capacity [kWh]; *S: nominal size [kW];*

P: electrical power [kW]; *Q: heat [kW];*

SOC: State of Charge [-]; *ṁ: mass flow rate [kg/s]*

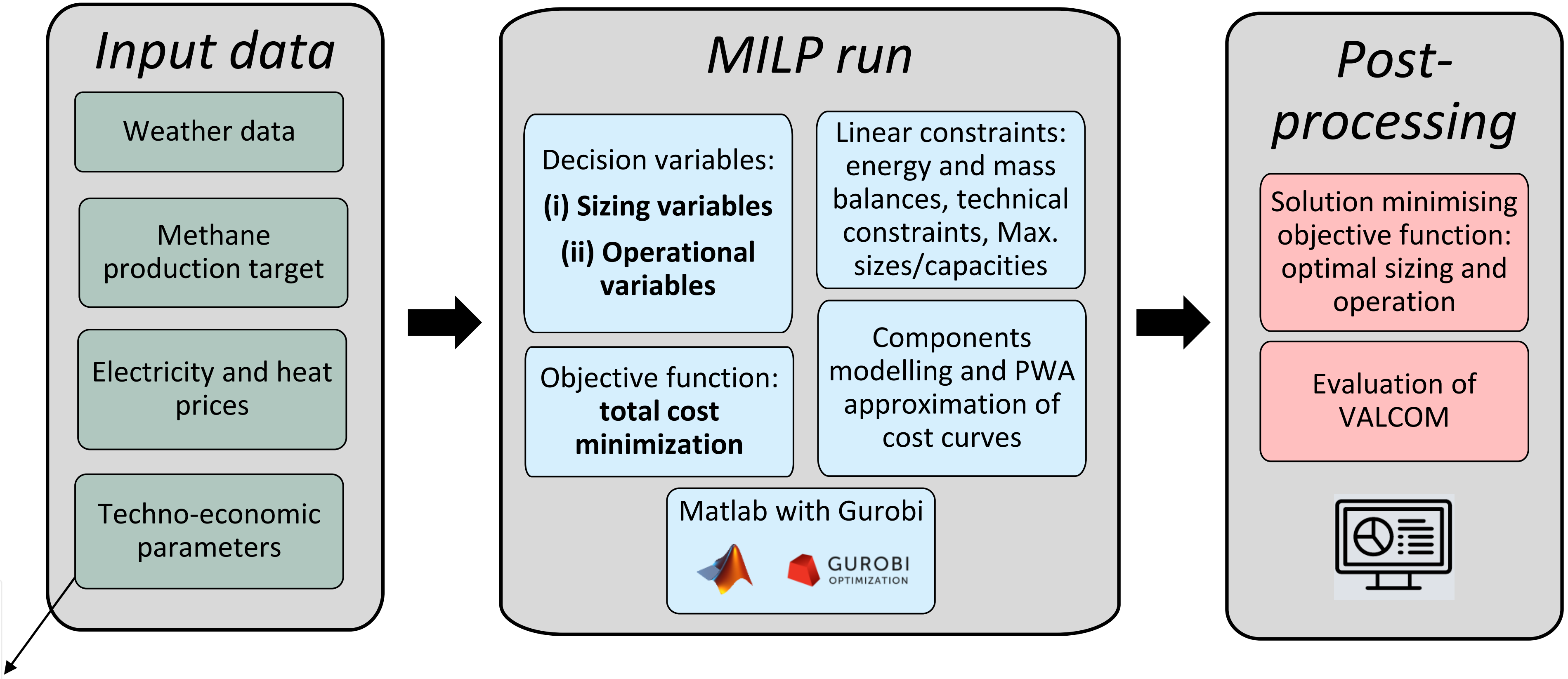
Boundary conditions

- The optimization approach considers a 1-year horizon and 1-hour resolution.
- As a case study, the year 2022 and the city of Zurich were considered.



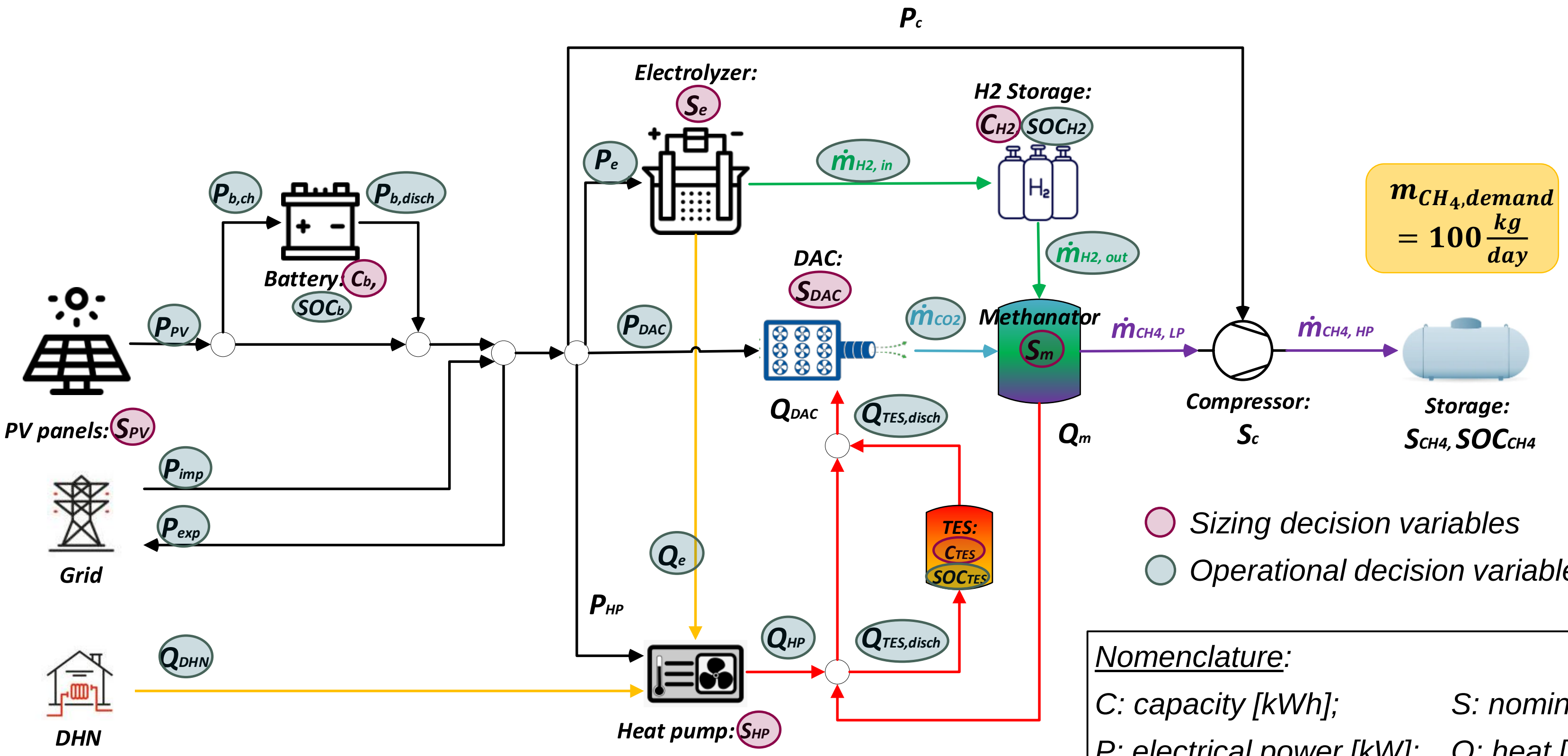
Design approach - MILP

- A deterministic mixed integer linear programming (MILP) approach was adopted.



VALCOM: value-adjusted levelized cost of methane

Decision variables – what can the optimizer decide



$$m_{CH_4,demand} = 100\,\frac{kg}{day}$$

Sizing decision variables

Operational decision variables

Nomenclature:

C: capacity [kWh]; S: nominal size [kW];

P: electrical power [kW]; Q: heat [kW];

SOC: State of Charge [-]; ṁ: mass flow rate [kg/s]

Objective function – what do we optimize for?

- For the selected location, techno-economic parameters and desired methane production rate, what are the sizing and operational variables to achieve minimal total cost?

$$\begin{cases} \min(cost_{tot}) \\ s.t.\, m_{CH4,day} > 100\,\frac{kg_{CH4}}{day} \\ Energy\ and\ mass\ balance \\ Operational\ and\ technical\ constraints \\ maximum\ componets'sizes \end{cases}$$

$$cost_{tot} = cost_{inv} + cost_{op} + cost_{maintance} + cost_{shut-down}$$

- ❖ $cost_{inv} = \sum_{i=1}^{\#components} S_i \cdot \frac{UP_i}{lifetime_i}$
- ❖ $cost_{op} = \sum_{n=1}^{8760} P_{imp}(t) \cdot cost_{el,imp}(t) - \sum_{n=1}^{8760} P_{exp}(t) \cdot cost_{el,exp}(t) + \sum_{n=1}^{8760} Q_{imp}(t) \cdot cost_{heat,imp}(t)$
- ❖ $cost_{maintance} = \sum_{i=1}^{\#components} S_i \cdot cost_{maintanace,\%}$
- ❖ $cost_{shut-down} = \sum_{j=1}^{\#shut-down} \frac{c_{shut-down,u}}{(length_{shut-down})^{1.5}}$ *[1]*

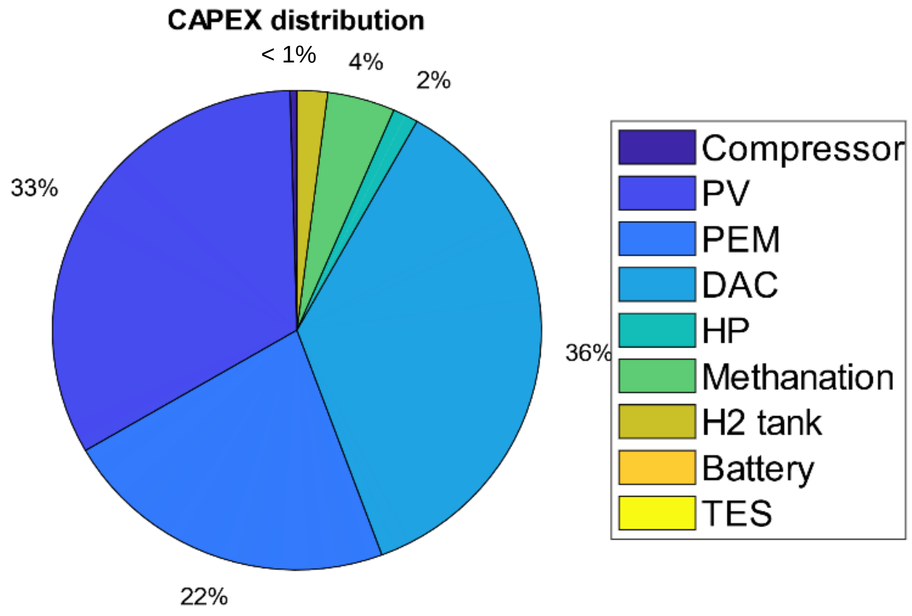
Value-adjusted levelised cost of methane

→ $VALCOM = \frac{cost_{tot} - cost_{shut-down}}{m_{CH4,year}}$

[1] Rioja et al., Applied Energy, 2022

Results – optimal sizing

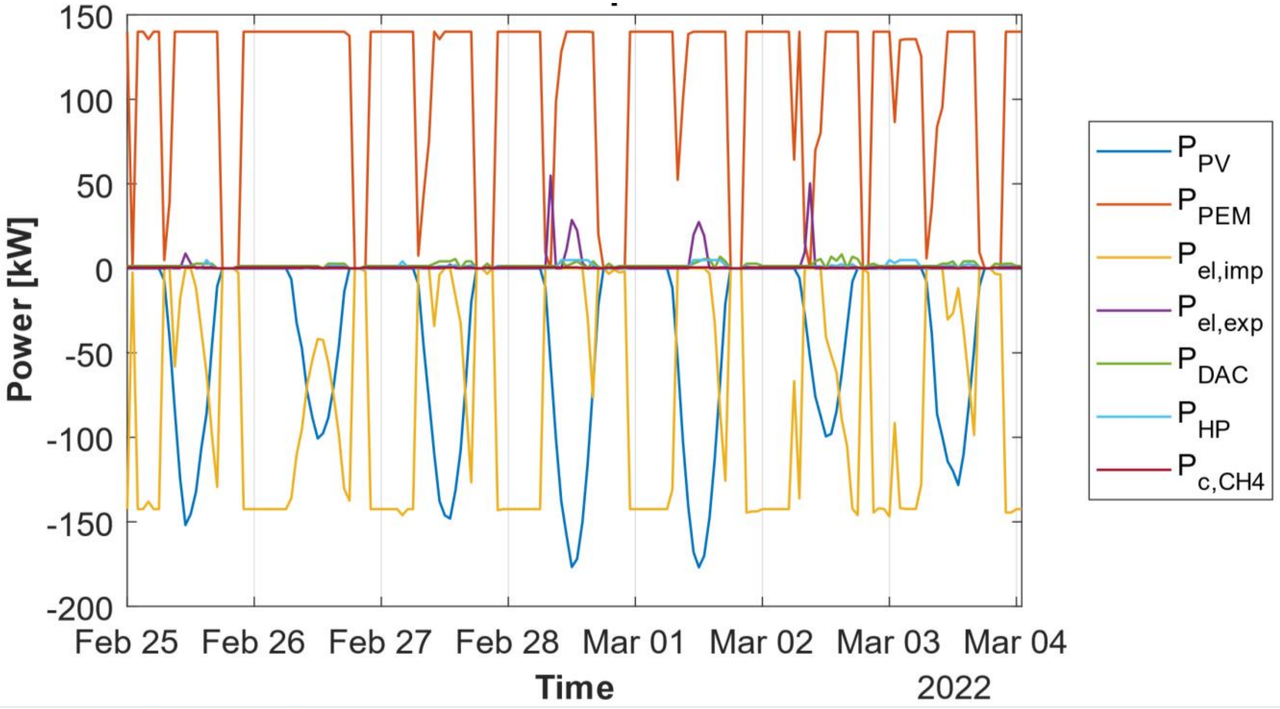
- Main CAPEX drivers are PV, PEM, DAC (91 %)
- Local PV generation is beneficial. **Available PV space has a large influence on VALCOM.**
- Compared to a case without waste heat recovery (WHR):
  - heat from DHN reduced by 82%;
  - Optimal sizes are slightly affected;
  - VALCOM reduced by 5.74%.



	S_{PV} [kW]	S_e [kW]	$\dot{m}_{CO2,nom}$ [kg_{CO2}/h]	$\dot{m}_{CH4,nom}$ [kg_{CO2}/h]	H2 tank [kWh]	Battery [kWh]	TES [kWh]	VALCOM [€/MWh]
with WHR	284.4 (max)	140	13.8	5.0	772 (+ 25%)	0	80 (max)	505.25 (-5.74%)
w/o WHR	284.4 (max)	140	13.8	5.0	617.6	0	80 (max)	534.23

Results – optimal operation

- Operational costs account for **71.8%** of total costs;
- Thanks to optimal thermal integration, costs for heat imports are almost null;
- Main **electricity** consumption from PEM electrolyzer:
  - DAC: 32.02 MWhel/year; PEM: 917.3 MWhel/year
  - When solar availability is high, electricity is imported at night and early morning.



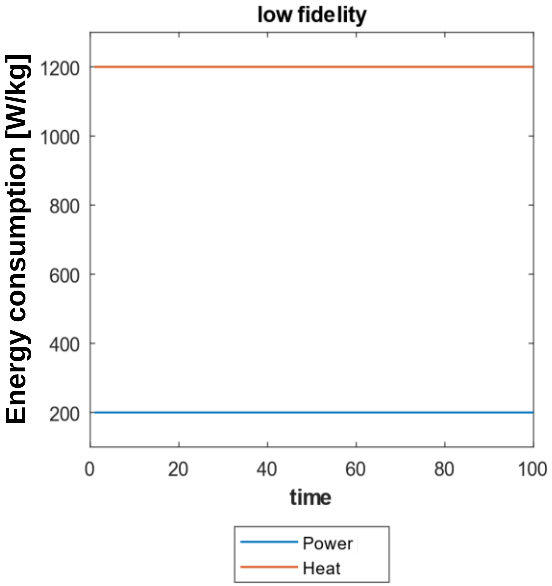
Impact of storage options

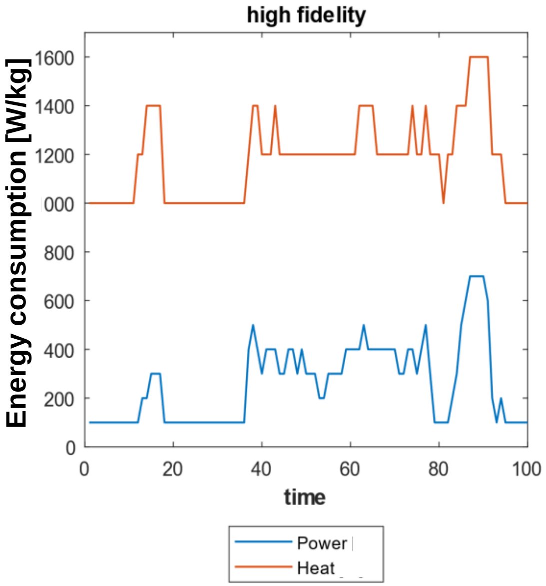
- **Accounting for storage options impacts the optimal sizing of conversion technologies**: PEM electrolyzer size increase by 16.7%;
- H2 tank and TES selected, while battery is not selected due to high investment costs;
- Operational costs are reduced, while investment cost slightly increased → **VALCOM reduced by 1.44%**

	No storage options available	Storage options available (battery, H2 tank, TES)	
PV [kW]	284.4 (max)	284.4 (max)	
PEM [kW]	120.0	140.0	+16.7%
DAC [kW]	16.5	16.5	
HEAT PUMP [kW]	28.9	29.0	
COMPRESSOR [kW]	0.5	0.5	
H2 tank [kWh]	0.0	772.0	
Battery [kWh]	0.0	0.0	
TES [kWh]	0.0	80.0 (max)	
VALCOM [€/MWh]	542.0	534.2	
difference	-	-1.44%	

Impact of DAC modelling level of fidelity

- Low-fidelity: constant consumption (based on average T and humidity);
- High-fidelity [1]: consumption as a function of weather data;
  - Low-fidelity model underestimaes VALCOM (difference of 3.37%);
  - Device sizing (number of units) remains unvaried in the example selected.

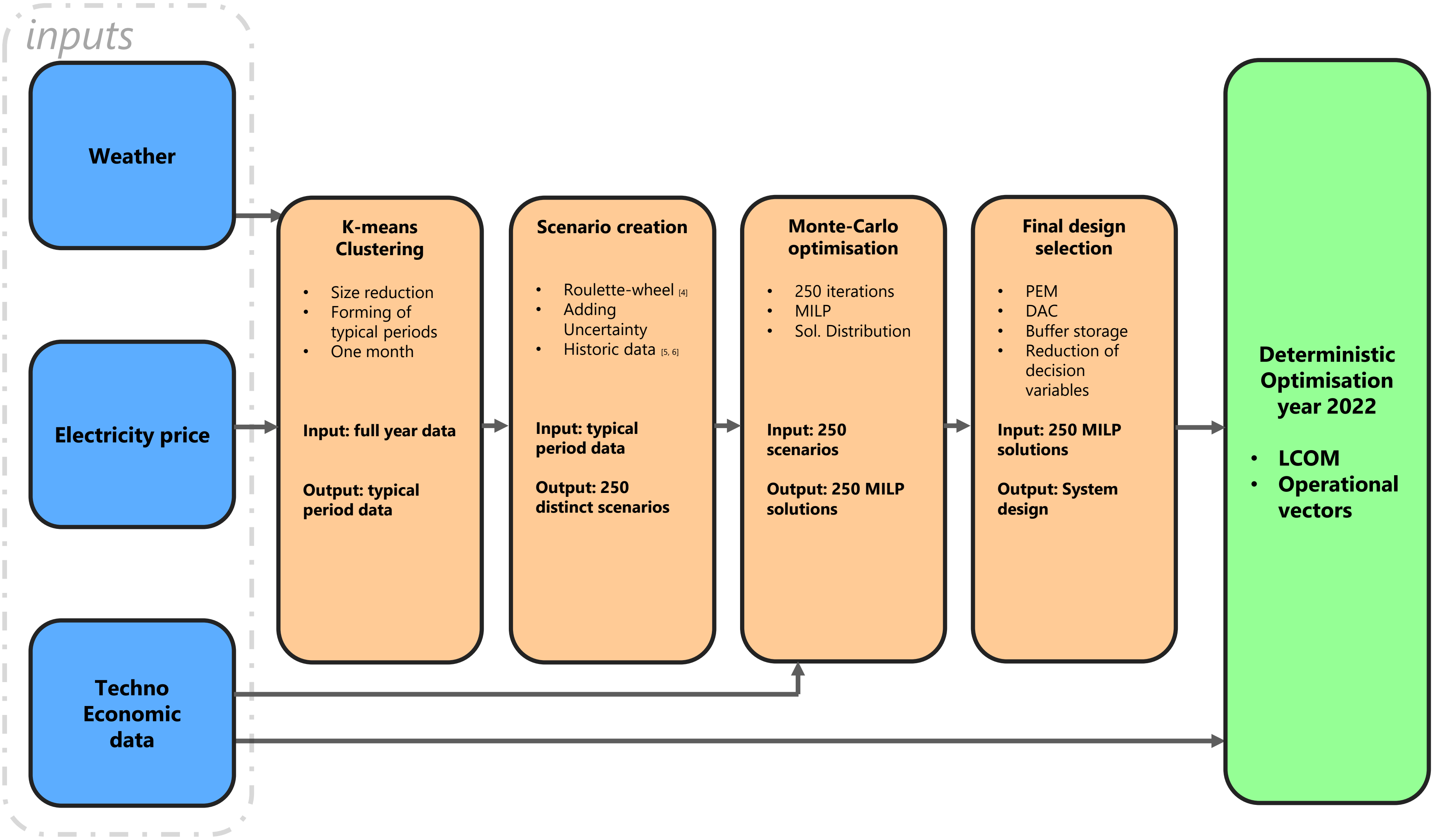




	VALCOM [€/MWh]
Low fidelity	488.76
High fidelity	505.25

[1] Wiegner et al., Optimal Design and Operation of Solid Sorbent Direct Air Capture Processes at Varying Ambient Conditions, 2022

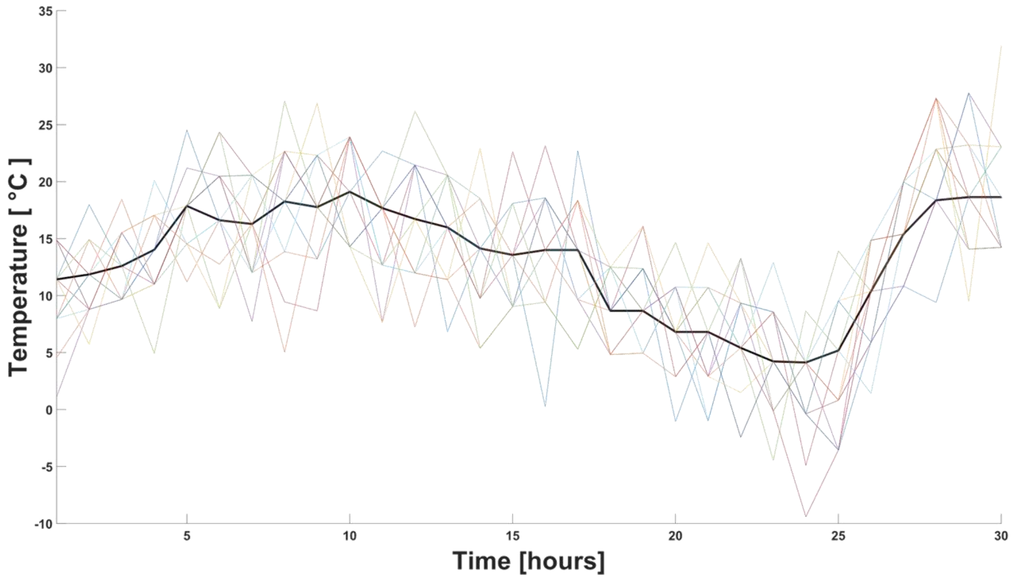
Accounting for uncertainty – Monte-Carlo optimization



Tim Müller, Optimal design of synthetic methane production site including device sizes and operating schedule, master thesis ETH, 2024

Monte-Carlo optimization – preliminary results

- Scenarios created using roulette-wheel [1] for: Irradiance, cost of energy, temperature, humidity;
- Currently, no correlations between parameters is considered, e.g. higher irradiance does not mean higher temperature.



- Results indicated the H2 tank as the most sensitive size;
- However, for the considered design case, no major differences were found compared to the deterministic case

Bat.	DAC	PEM	TES	H2
0 kWh [100 %]	13.75 kg/h [100 %]	140 kW [100 %]	70 kWh [86 %]	Variable

# modules	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Occurencies	1	5	9	24	29	32	39	28	25	23	18	8	7	2

Each module stores 70 kWh of H2

Results from Tim Müller, Optimal design of synthetic methane production site including device sizes and operating schedule, master thesis ETH, 2024

[1] Emanuela Marzi et. al.: Power-to-Gas for energy system flexibility under uncertainty in demand, production and price

Synthetic methane production at Empa: move-mega

- Empa hosts a demonstrator for the future of mobility: move;
- The site hosts a 180 kW PEM electrolyzer. Hydrogen is stored up to 900 bar;
- The move-mega project will expand the current demonstrator by the addition of DAC unit from climeworks and an innovative methanator concept [1];
- The goal is to monitor performance in a real-world scale and to develop and test control strategies [2] to maximize hydrogen and methane production;

Move @Empa

Move-mega

[1] Kiefer et al., Sorption-enhanced methane synthesis in fixed-bed reactors, 2023
[2] Barbaresi et al., Partial-Load and Dynamic Operation of Methane Synthesis Reactors Using Sorption-Enhanced Catalysis, 2024

Key takeaways

- Optimal solution is highly sensitive to input parameters, which needs to be selected carefully;

- Operational costs are the dominating cost factor and are mainly dictated by the imported electricity to operated the PEM electrolyzer. The main CAPEX are linked to PV, PEM electrolyzer and DAC;

- The use of storage options impact the optimal sizing of conversion technologies.

- Optimal thermal management reduces VALCOM of 5.74%, with a 82% reduction in imported heat compared to design solutions without waste heat recovery.

Reflections and future research directions

- **Design of energy systems:**
  - The uncertainty linked to input parameters and boundary conditions need to be considered during the design phase to generate robust ‘optimal’ design;
  - More accurate operational constraints needs to be included in the design problem to reduce the gap between design and operational stages and avoid suboptimal operation;

- **Synthetic methane:**
  - Need to reduce investment costs for H2 and CO2 production technologies;
  - Operational costs for electricity are high; economic viability depends on RES availability;

- **Hurdles for DAC:**
  - Lack of in-field data and unit prices;
  - Investment costs are still high;
  - Need for life cycle assessment;

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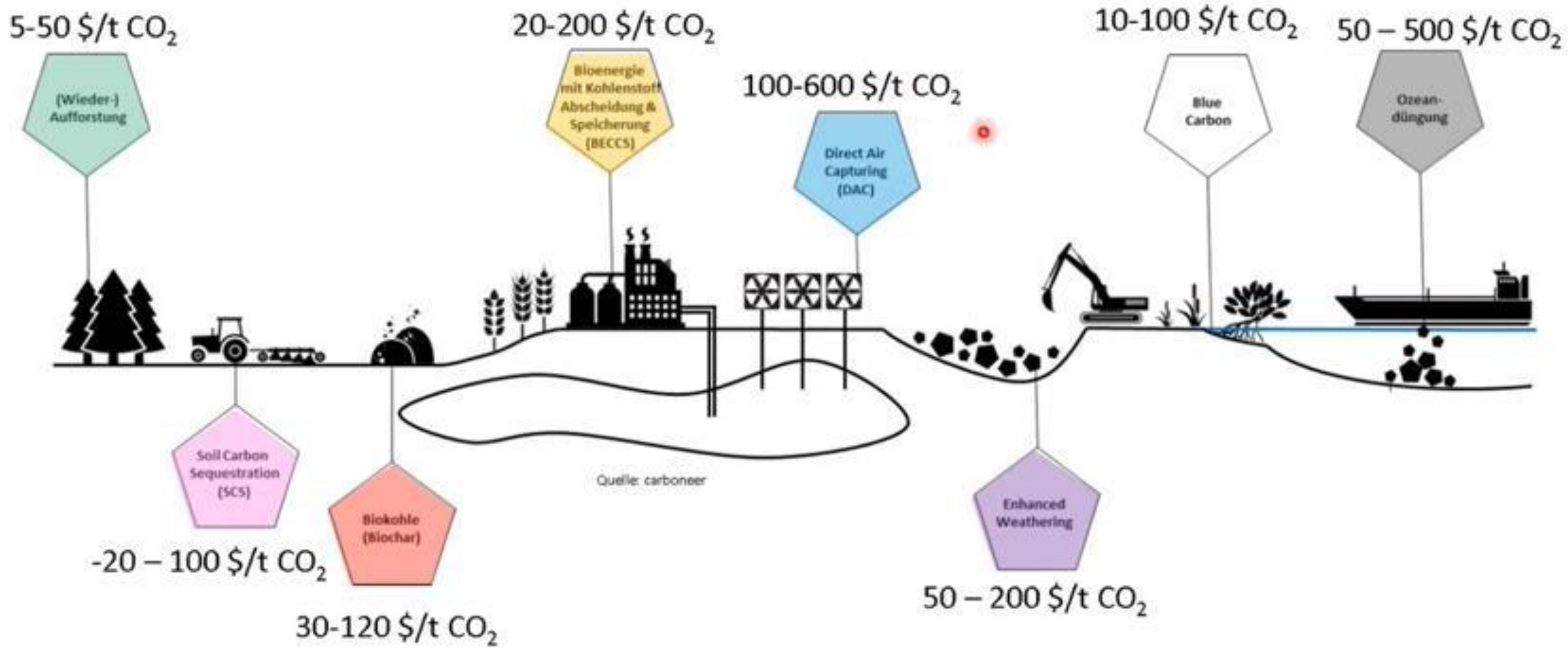
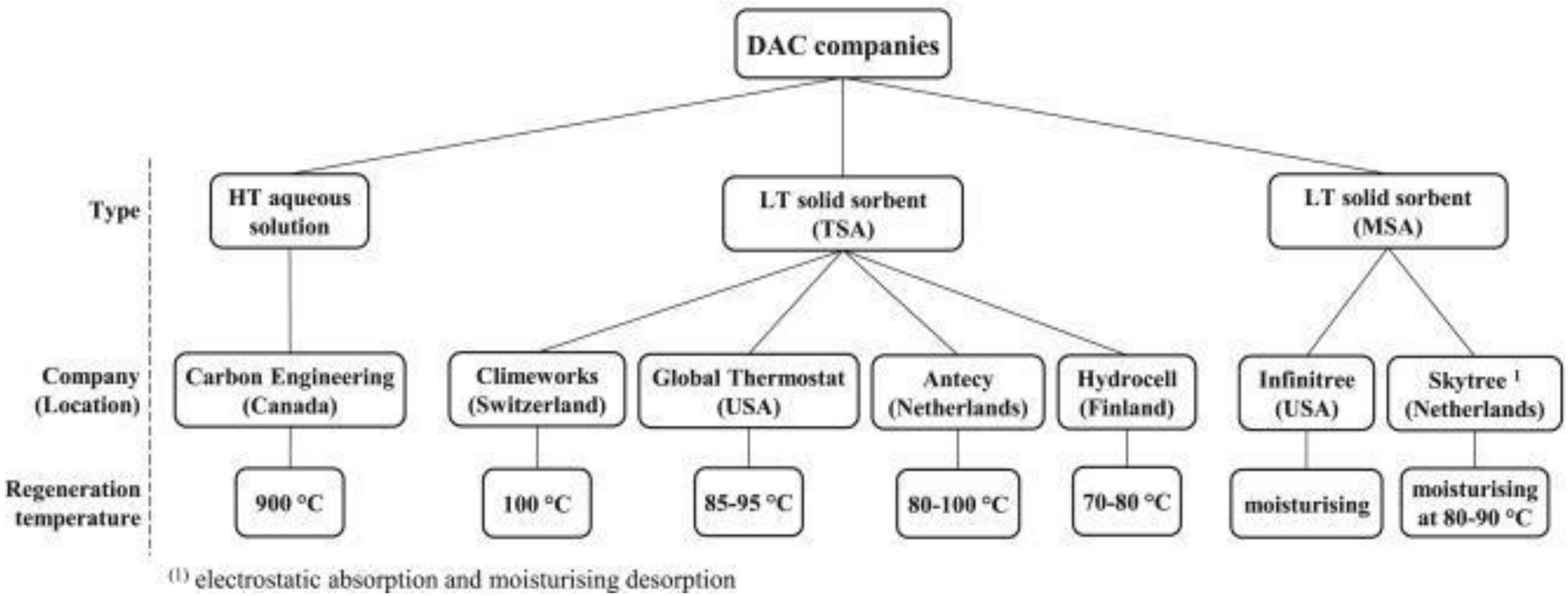
CO2 costs



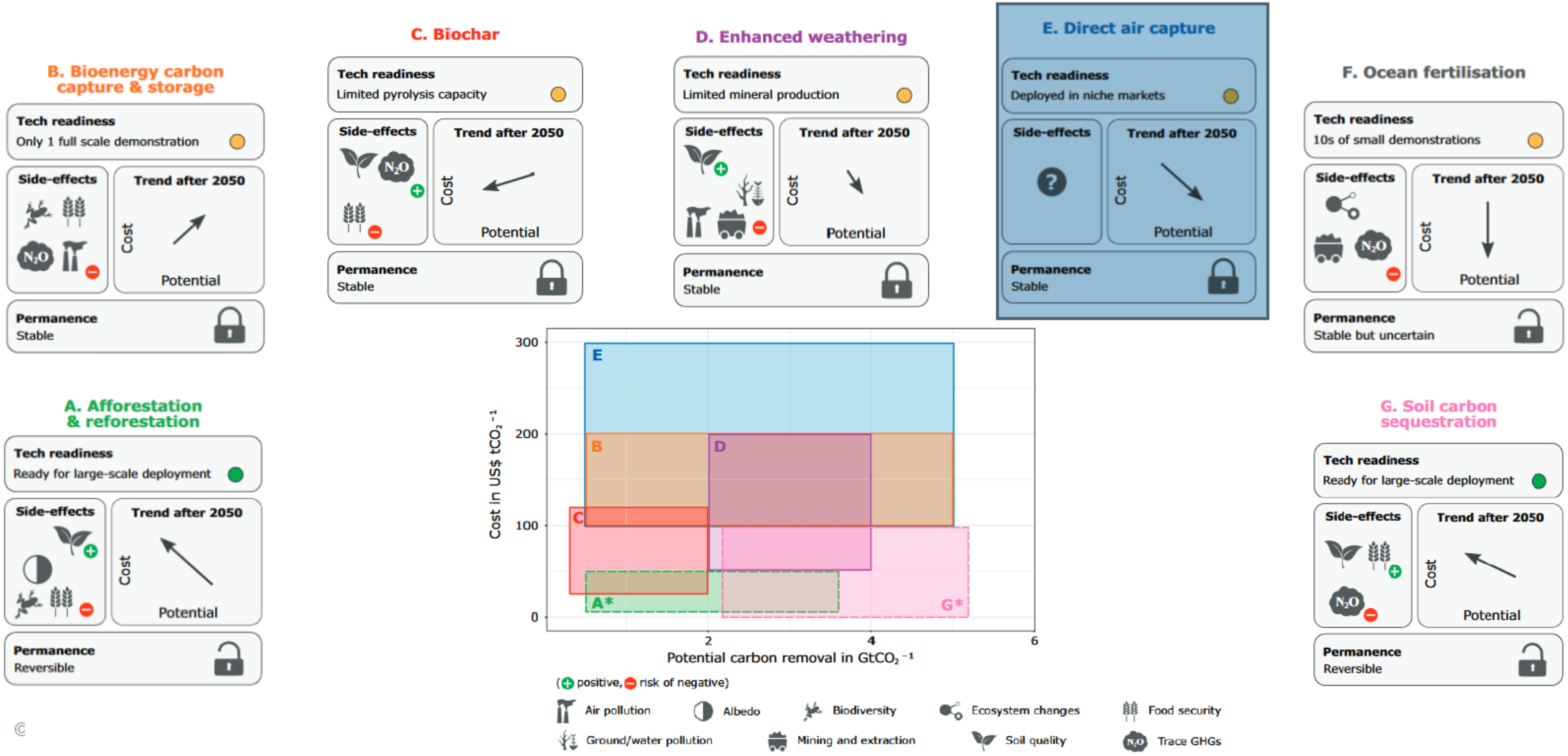
Carboneer.earth.com

DAC companies



M. Fasihiet al. J. Clear Prod., 224, 957-980, (2019), H. McLaughlin et al. Renewable Sustainable Energy Rev., 177, 113215 (2023)

The role of negative emissions technologies



Courtesy of Dr. Marc Vocht

Cost of storage

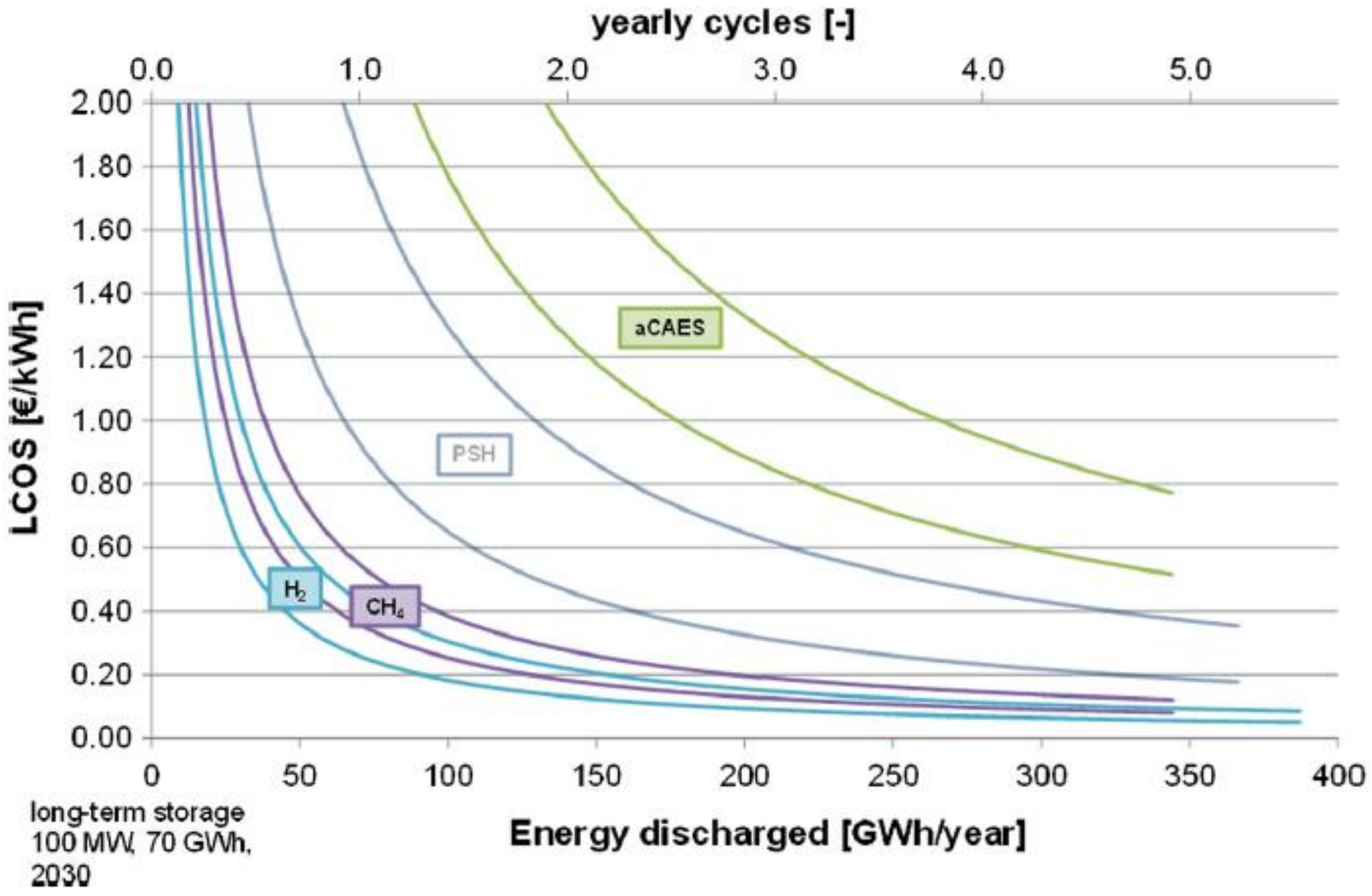


Fig. 2. LCOS for long-term storage systems in 2030 depending on the yearly energy discharge, not including cost of electricity.

Julch, Comparison of electricity storage options using levelized cost of storage (LCOS) method, 2016

Trends for the costs of key technologies

- Investment costs are expected to reduce by +50% in the next 20 years;
- These trends follow the typical learning curves of energy technologies;

Table 2. Average investment costs for the core components of PtG: alkaline and membrane electrolysis (alkaline, membrane (PEM)) and methanation (chemical, biological) for the MW class. The kW unit refers to the electrical power input of the electrolysis, not the gas flow rate [3].

Year	Alkaline Electrolysis in EUR/kW	Membrane Electrolysis in EUR/kW	Chemical Methanation in EUR/kW	Biological Methanation in EUR/kW
2010	1150	1650	1040	1600
2015	980	1350	870	1300
2020	850	1130	740	1050
2025	720	950	620	860
2030	620	780	520	690
2040	460	530	370	460
2050	330	350	260	300

Sterner et al., Power-to-Gas and Power-to-X—The History and Results of Developing a New Storage Concept, 2021

Table 4. Reported learning rates of selected technologies.

Technology	LR	Source
Lithium-ion batteries (electronics)	30%	[69]
Solar PV	23%	[68]
LED A lamps	18%	[71]
Natural gas turbines	15%	[68]
Hydraulic fracturing	13%	[76]
Onshore wind	12%	[68]
Nickel-metal hydride HEV batteries	11%	[69]
Flue gas desulfurization systems	11%	[77]
PC coal boilers	5.6%	[78]
Hydroelectric power	1.4%	[68]

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Costs for DAC

Table 2. Literature cost estimates for solid sorbent DAC.

	Sinha *et al*[a] [19]	Sinha and Realff[b] [19]	NASEM[c] [2]	McQueen *et al*[d] [32]
Gross cost projection ($ tCO_2^{-1})	—	86–221	88–229	Base case: 223 Geothermal: 205 Nuclear: 233
Net removed cost projection ($ tCO_2^{-1})	—	—	124–407	—[d]
Scale ($MtCO_2\ yr^{-1}$)	—	1	1	0.1
Plant economic lifetime (years)	10	10	10	10
WACC	—	—	0%	12.5%
Electricity resource (cost)	Source agnostic (-)	Source agnostic ($0.06 kWh^{-1})	Natural gas ($60 MWh^{-1})	U.S. grid ($0.06 kWh^{-1})
Thermal energy resource (cost)	Steam (-)	Steam ($0.0015 kg^{-1})	Natural gas ($3.25 GJ^{-1})	Base case steam ($2.8 GJ^{-1}) Geothermal waste heat ($0.00 GJ^{-1}) Nuclear slip steam ($3.90 GJ^{-1})
Sorbent material	MIL-101(Cr) mmem-Mg_2(dpbpdc)[e]	Specific sorbent material not specified	Specific sorbent material not specified	Specific sorbent material not specified
Sorbent lifetime (years)	—	0.5	0.5	1
Sorbent capacity ($mol\ kg^{-1}$)	1 2.9	—	1	1
Adsorption process	TVSA	TVSA	TVSA	TVSA
Cycle time (min)	40 75	15–85	16, 28, 42	20
Desorption temperature (°C)	100	87	87	100
Desorption swing capacity ($mol\ mol^{-1}$)	—	0.8	0.8	0.8
Includes CO_2 compression?	No	No	No	No

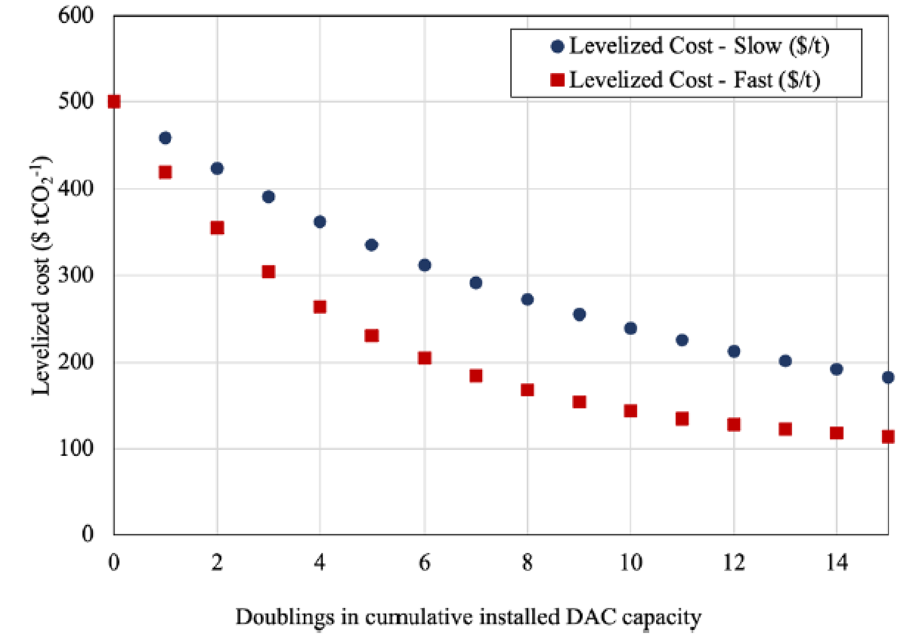

Figure 3. Projected levelized cost of DAC as a function of the number of doublings in the cumulative installed DAC capacity (in $tCO_2\ yr^{-1}$). Levelized cost is the sum of lifetime capital and operating costs divided by the lifetime tonnes removed.

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