



DACS Talk 1

Ventilation-integrated Direct Air Capture

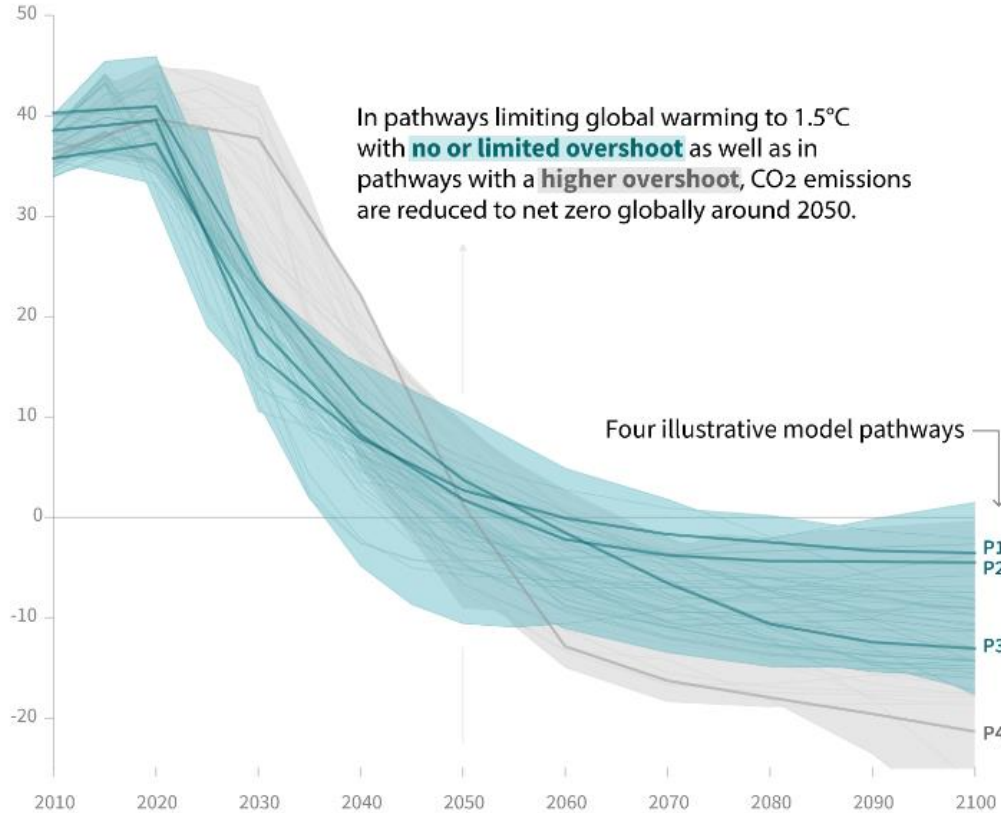
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06.12.2023

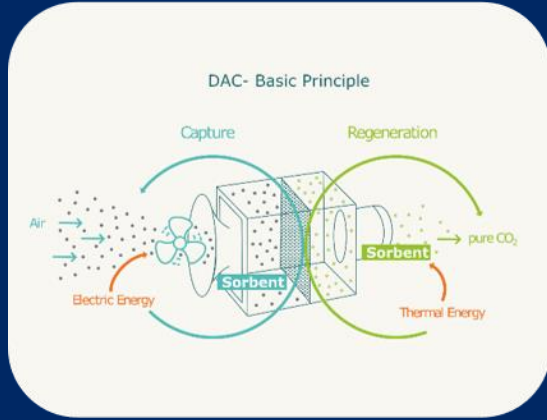
Global total net CO₂ emissions

Billion tonnes of CO₂/yr

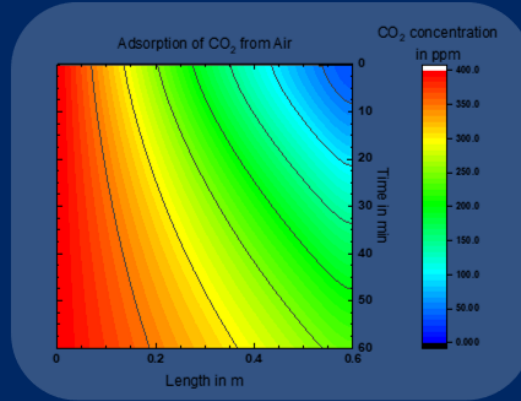


CO₂ emissions must be reduced below zero to reach the 1.5°C goal!
Direct Air Capture (DAC) can help with both!

DAC- Principles



Modelling



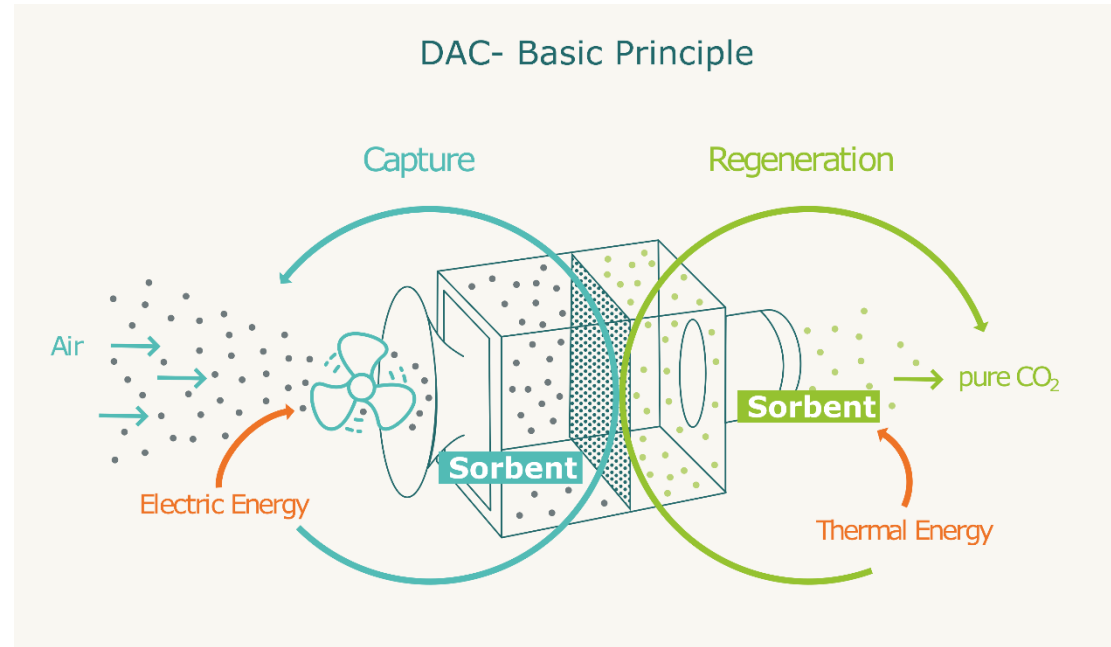
Arginine System



Agenda

Basic Principle of Capture and Regeneration for Direct Air Capture (DAC)

- DAC is a cyclic process, consisting of capture and regeneration
- While capture a specialized filter material is contacted with air and binds the CO₂ on the surface of a solid (Adsorption) or in a liquid (Absorption)
- The CO₂ can be released by energy input (either heat or electricity)



Different DAC principles and performances

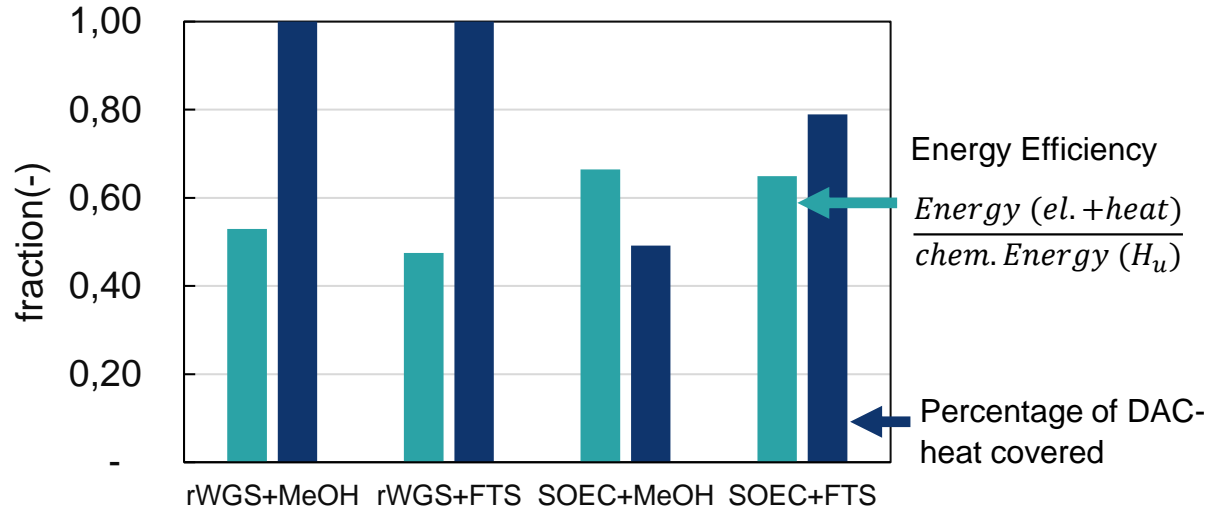
- Main Energy demand is heat for LT and HT-DAC
- LT-DAC (solid sorbent): Steam with 100°C
- HT-DAC (liquid sorbent): 900°C heat with natural gas burners
- Both are at TRL8 with pilot plant operating or in construction
- Novel approaches (e.g. Electro-Swing-Adsorption)

Technology		HT-DAC	LT-DAC	ESA
Energy demand (MWh/t _{CO2})	Electr.	0.36	0.2-0.3	0.25-0.5
	Thermal	1.45	1.2-2.0	0
Cost [today] (USD/t _{CO2})		64-232 [<250]	<100 [200-800]	50-100



Heat integration of LT-DAC with synthetic fuel production

- Process simulation using Aspen with hydrogen production and product synthesis
- Syngas production via Co-electrolysis in a solid-oxide fuel-cell (SOEC) or via reverse-water-gas-shift (rWGS)
- Product is Methanol (MeOH) or Fischer-Tropsch-Product (FTS)



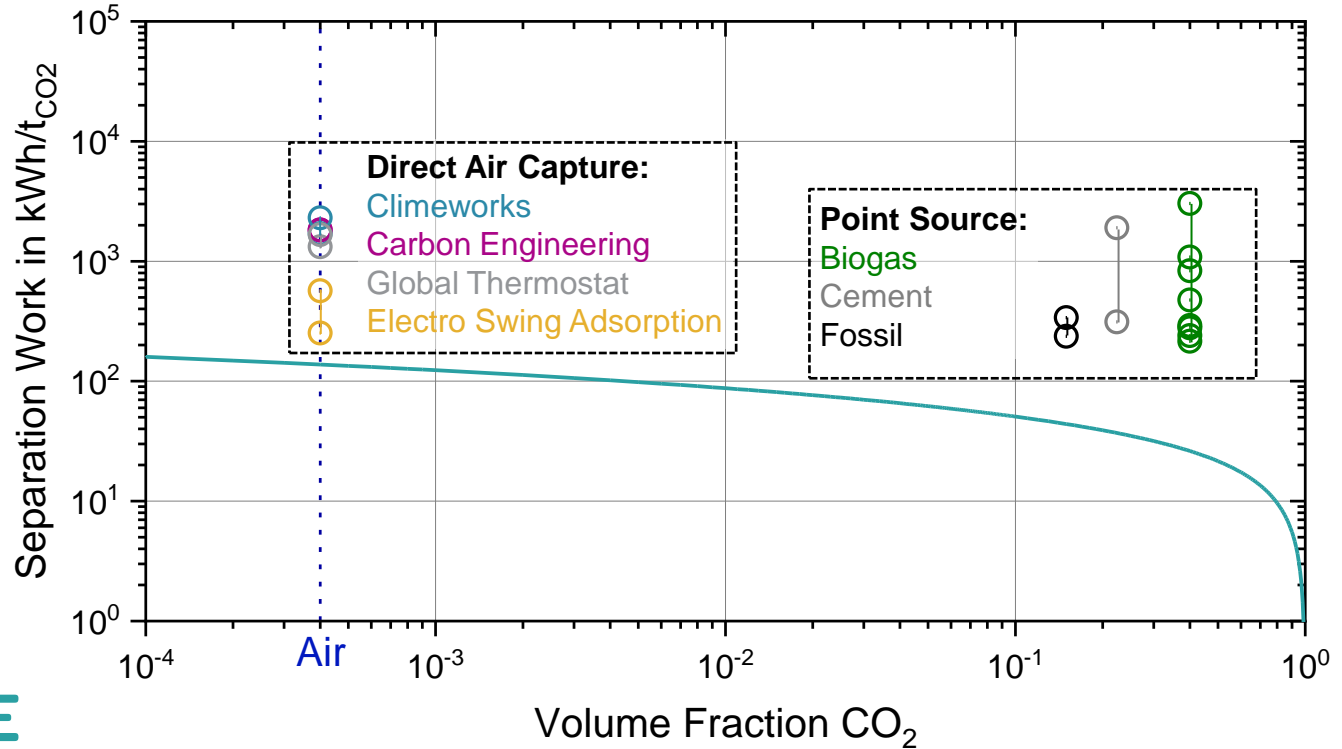
From: Heß, Dominik; Klumpp, Michael; Dittmeyer, Roland (2020): Nutzung von CO₂ aus Luft als Rohstoff für synthetische Kraftstoffe und Chemikalien. Hg. v. Verkehrsministerium Baden-Württemberg



A substantial percentage of the heat can be obtained from the conversion processes

Minimal thermodynamic Separation work of CO₂ from air

- There is a lower limit on how efficient DAC can get
- Novel DAC approaches promise to get close to this physical limit



Crowd Oil: Integrating DAC in ventilation systems

- Crowd Oil concept: HVAC-integrated DAC-units, to use existing air movement and infrastructure
- Utilization of waste heat and local renewable energy sources to spread the load on the energy system
- Numerous private investors could participate in the market of negative emissions
- Potential in Germany: Realistic potential of capturing 17 Mt CO₂ per year¹ by utilizing the ventilation capacity of large office and retail buildings



Picture: adapted from Dittmeyer et al 2019: Crowd oil not crude oil.

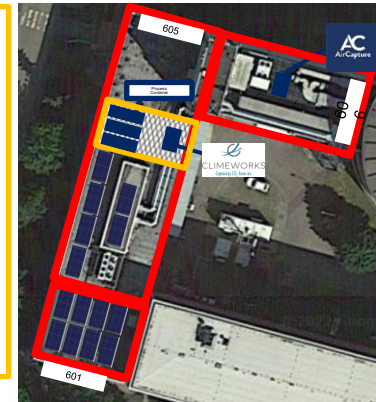
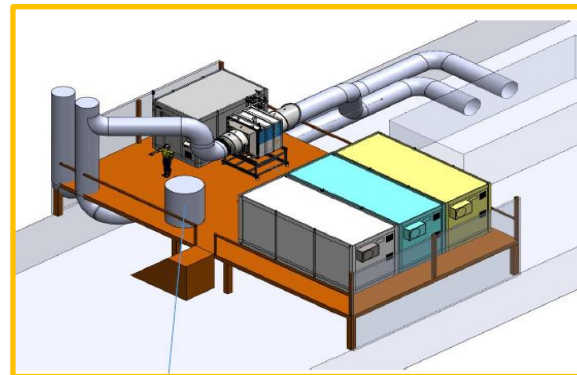
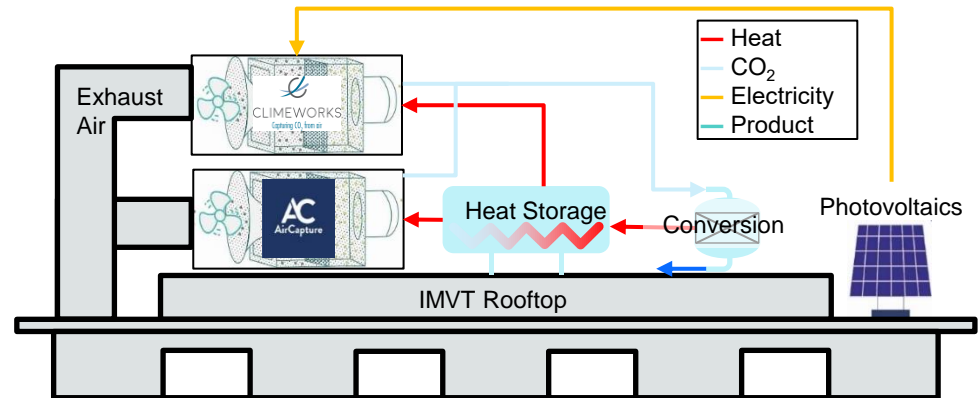
¹Mengis, Nadine et al. (2022): Net-Zero CO₂ Germany—A Retrospect From the Year 2050. In: *Earth's Future* 10 (2). DOI: 10.1029/2021EF002324.

Distributed DAC- The Rooftop lab at IMVT

Practical execution of the Crowd Oil Concept at the rooftop of IMVT



- Two different DAC units in the exhaust and input of the ventilation system
- Use of renewable energy and waste heat for direct air capture and utilization at the institute
- Goals:
 - Validation of HVAC-integrated industrial DAC units
 - Optimal layouts of HVAC-integrated DAC
 - Various operational strategies of HVAC-DAC
 - Explore real world obstacles for the successful integration of DAC in ventilation systems
- CO₂ utilization by ethanol synthesis



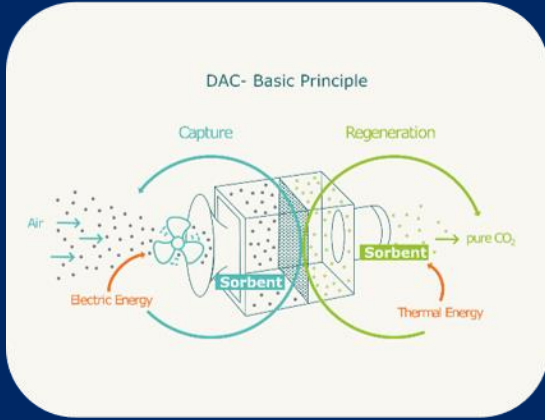
Next Level Ramp Up of
Direct Air Capture and Storage

DACStore

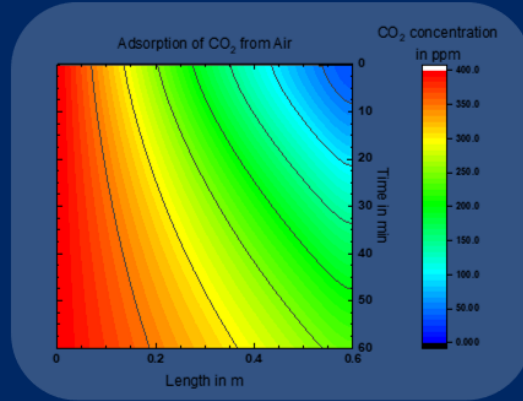
Impressions of the Rooftop Lab at KIT- IMVT



DAC- Principles



Modelling



Arginine System

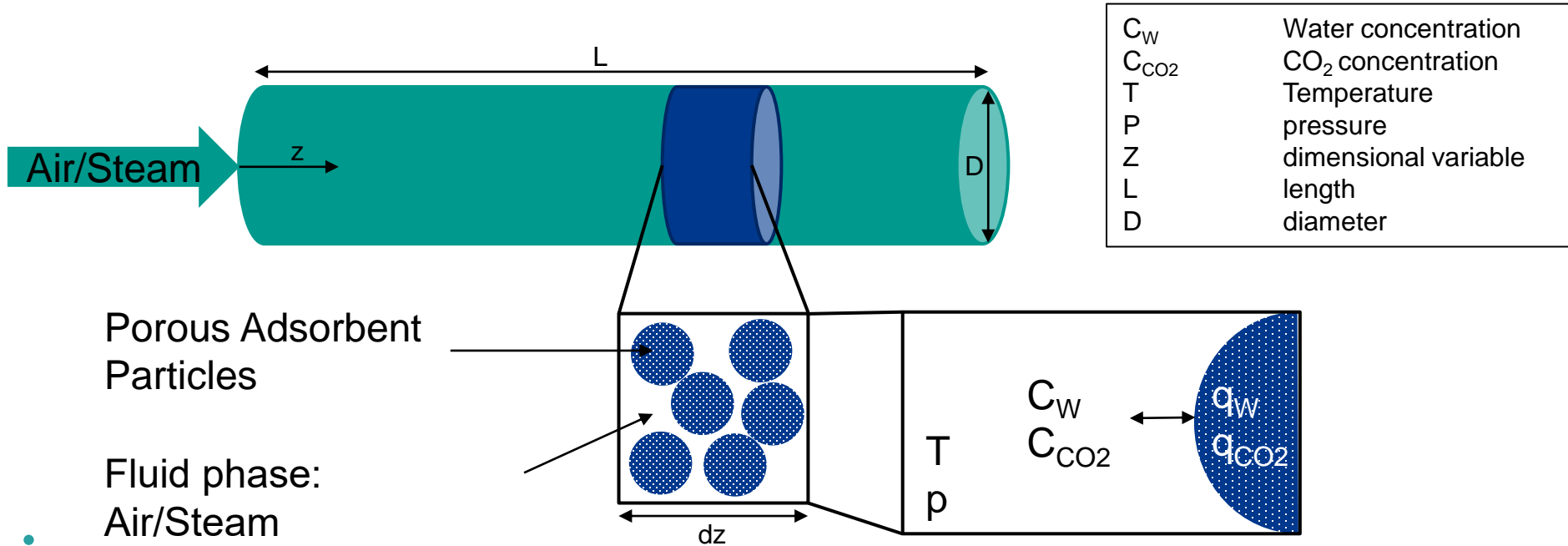


Agenda

Adsorber modelling: General Assumptions

- LT-DAC: Direct steam injection as regeneration method
- Fixed bed of round porous particles: Plug flow behaviour (1d model)
- Linear driving force- model: $\frac{\delta q_i}{\delta t} = K_{G,i}(q_i^* - q_i)$
- Multicomponent adsorption of water (GAB-isotherm) and CO₂ (Toth-isotherm) with co-dependent adsorption
- Thermal equilibrium, adiabatic, constant gas density, ideal gas behaviour
- Material balances: $\frac{\partial c_i}{\partial t} + u \frac{\partial c_i}{\partial z} - D_{ax} \frac{\partial^2 c_i}{\partial z^2} + \frac{\rho_{bulk}}{\epsilon_p} \frac{\partial q_i}{\partial t} = 0$
- Energy balance: $(\epsilon \rho_f c_{PF} + (1 - \epsilon) \rho_s c_{PS}) \frac{\partial T}{\partial t} = k_{fe} \frac{\partial^2 T}{\partial z^2} + (1 + \epsilon) \sum_i (-\Delta H_{ads}) \frac{\partial q_i}{\partial t} \rho_s$

Adsorber model: Cell method



C_w	Water concentration
C_{CO_2}	CO ₂ concentration
T	Temperature
P	pressure
Z	dimensional variable
L	length
D	diameter

Porous Adsorbent
Particles

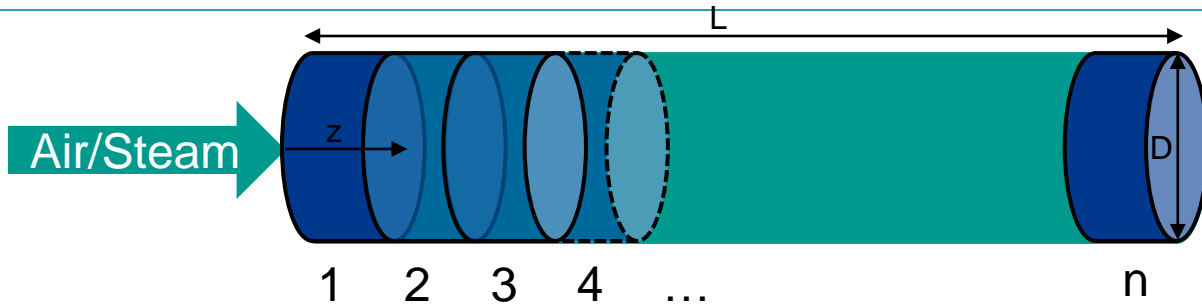
Fluid phase:
Air/Steam

Next Level Ramp Up of
Direct Air Capture and Storage

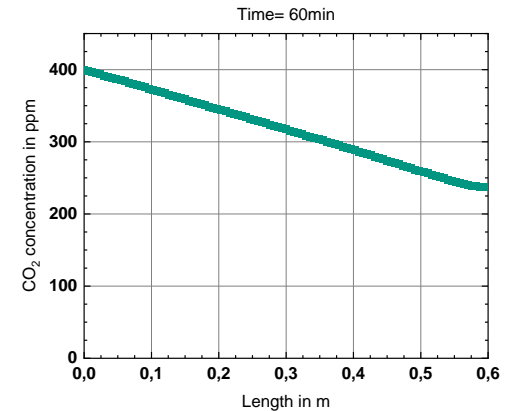
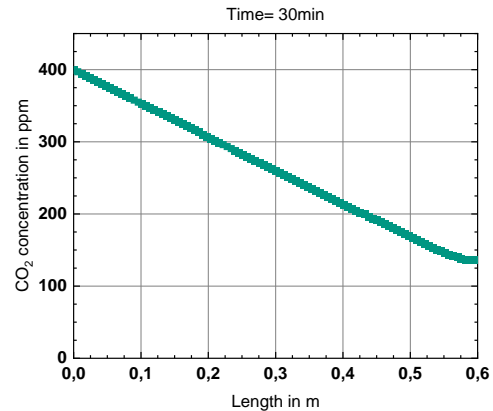
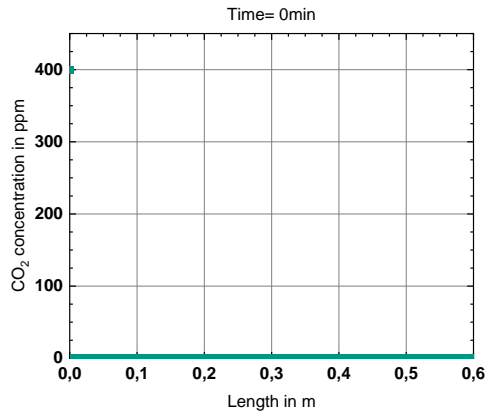
DACStorE



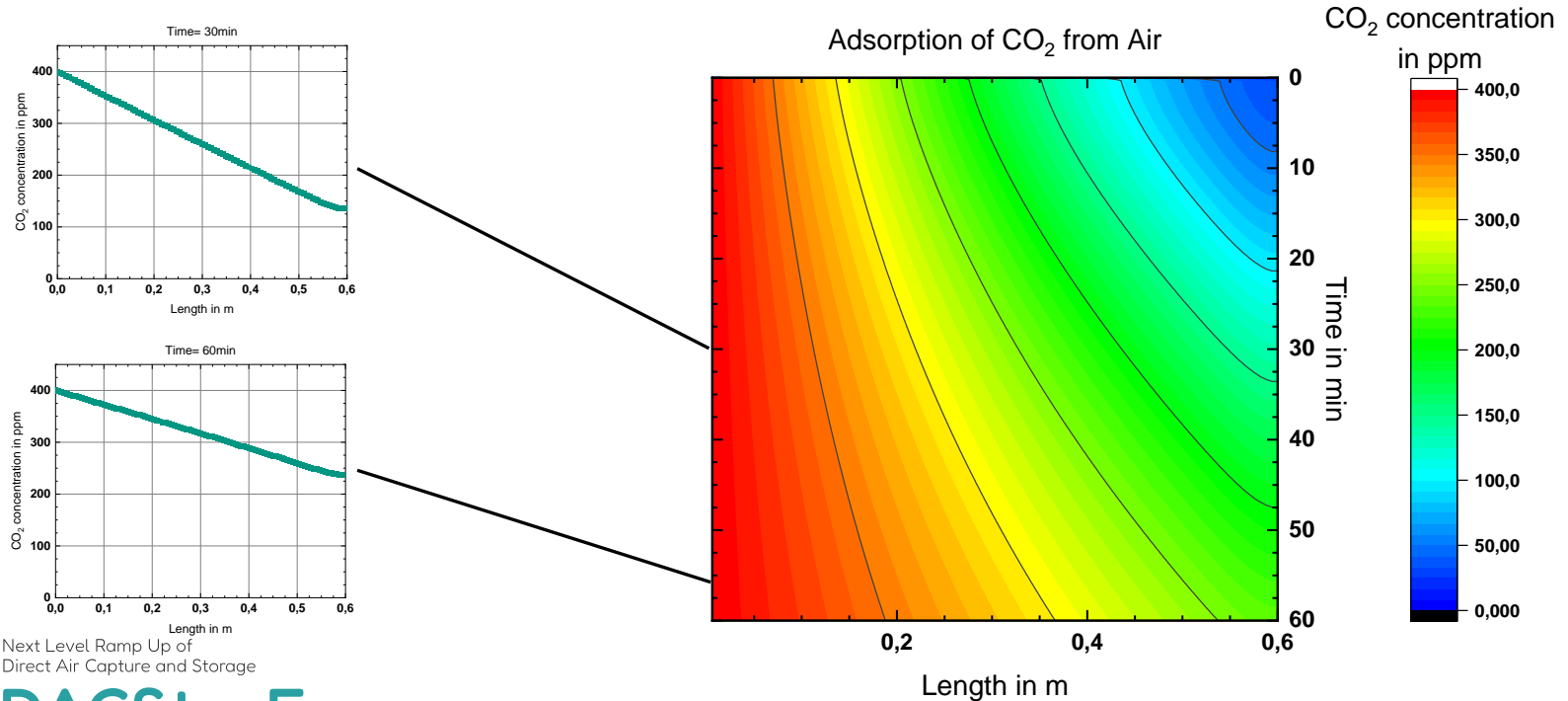
Adsorber model: Cell method



$$\begin{aligned}L &= 0,6\text{m} \\D &= 1,8\text{m} \\ \dot{V} &= 11000\text{m}^3\text{h}^{-1} \\T &= 20^\circ\text{C} \\p &= 1\text{atm} \\RH &= 0,4\end{aligned}$$

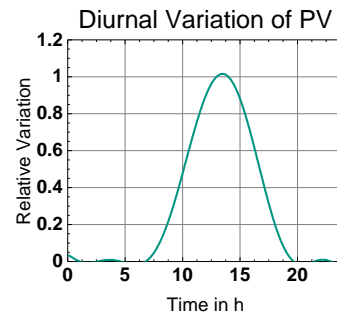
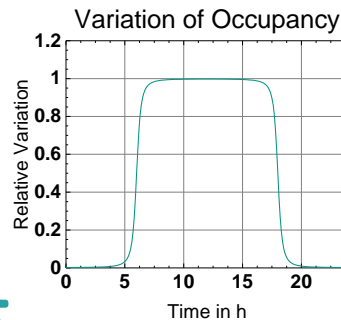
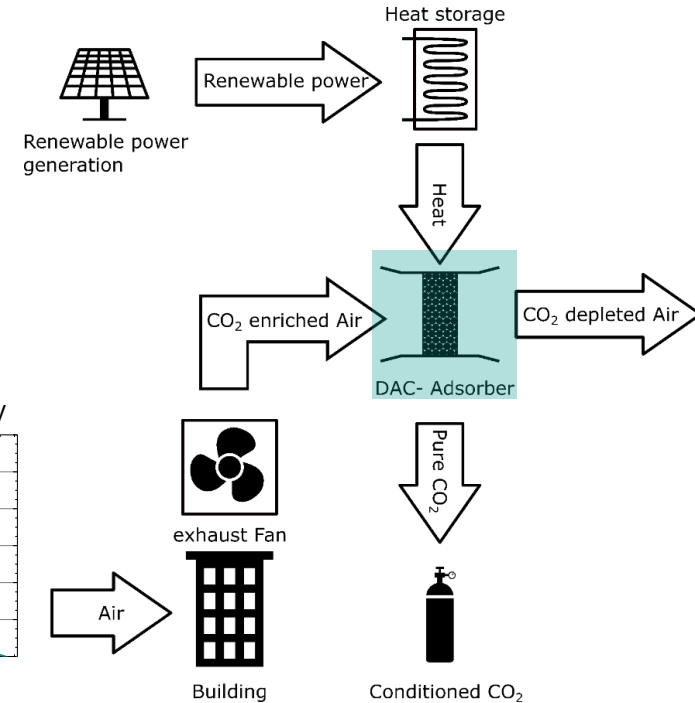


Output of the model: Continuous data of the adsorber state

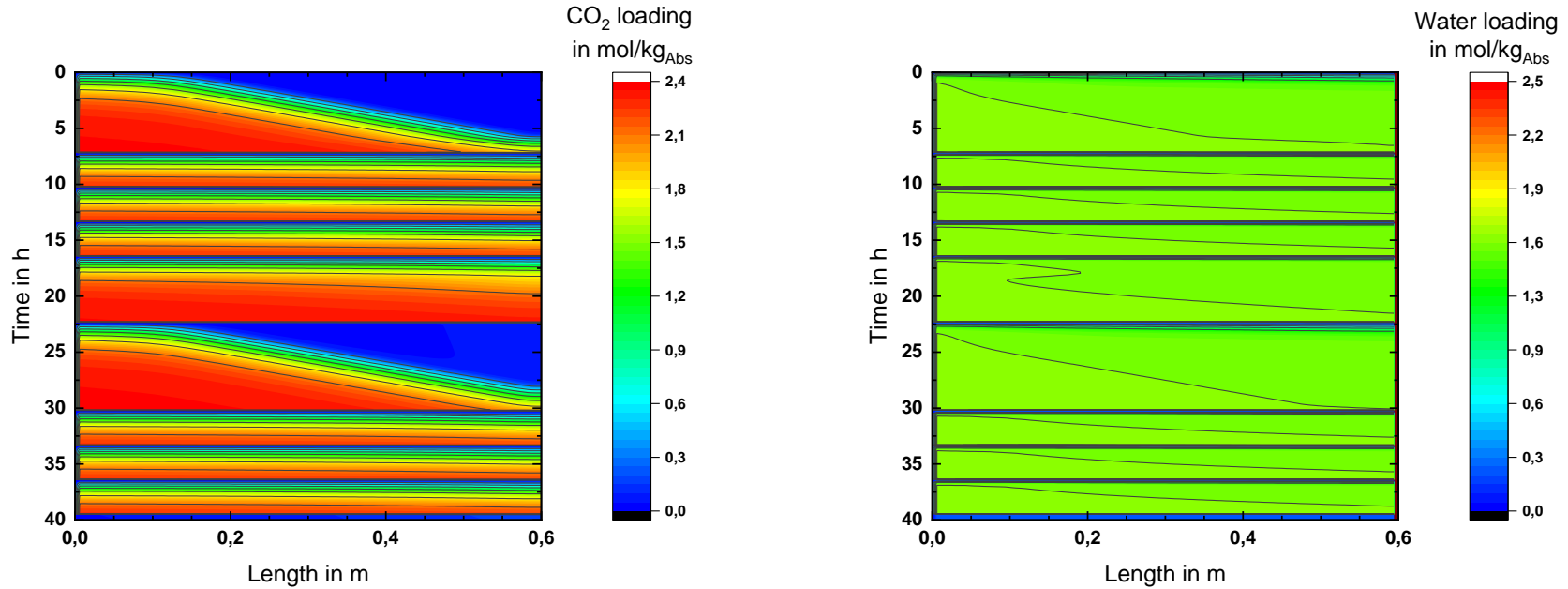


Distributed DAC- simulation of an integrated system

- Implementation of the Adsorber Model into a flowsheet simulation (Simulink)
- The system consists of:
 - Energy system: PV (diurnal variation), Heat Storage
 - Building: diurnal occupancy, varying CO₂ concentration
 - Fan: controlled or constant flowrate
 - Air intake: weather depended conditioned
- Dynamic inputs create complex output timelines

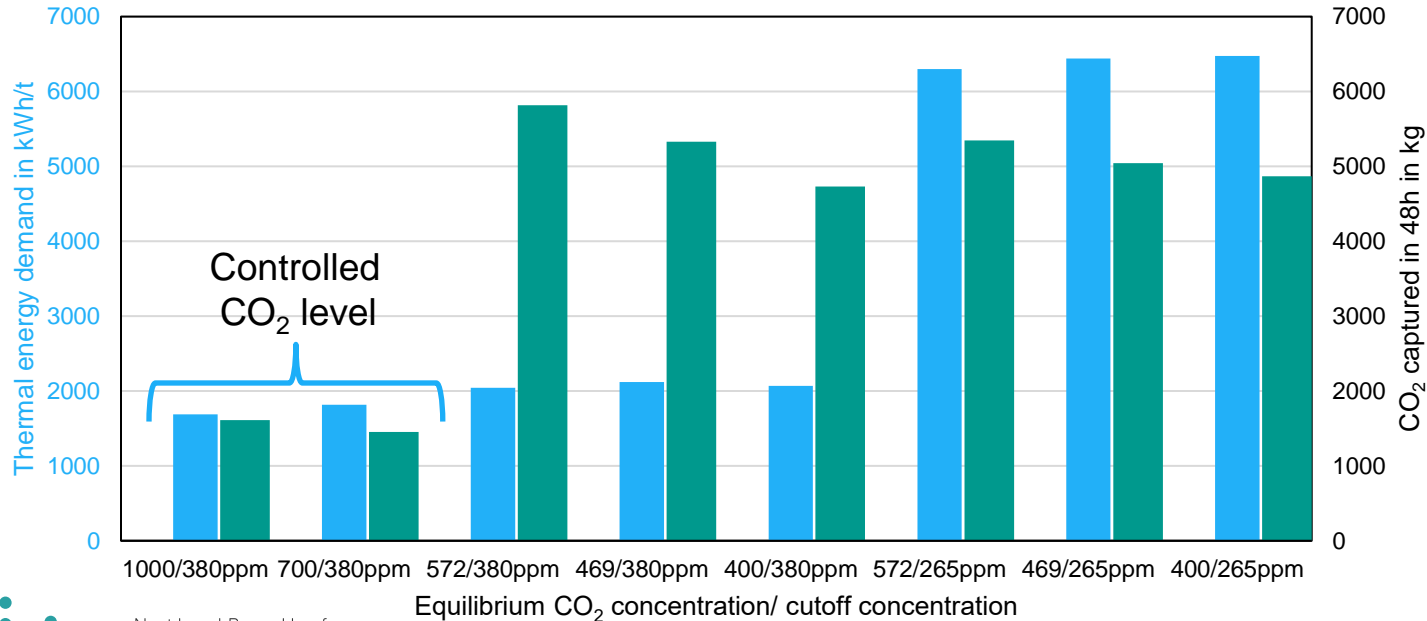


The flowsheet simulation gives a timeline of the adsorber



$T_{IN}=20^{\circ}\text{C}$, $\text{RH}=40\%$

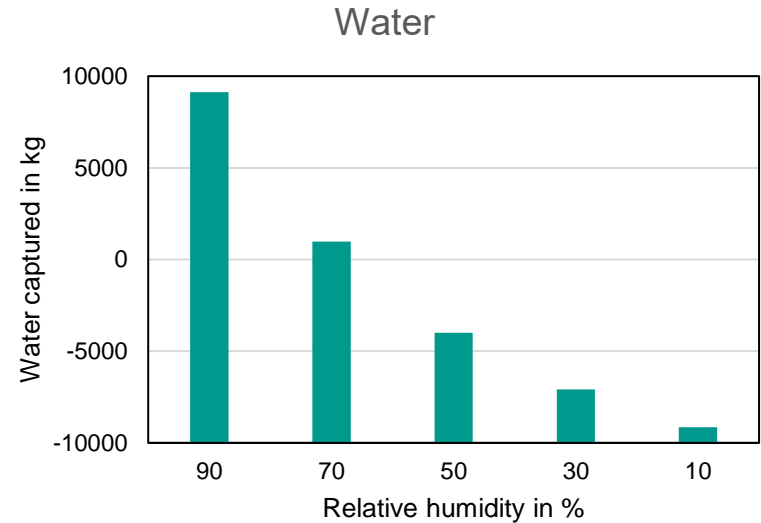
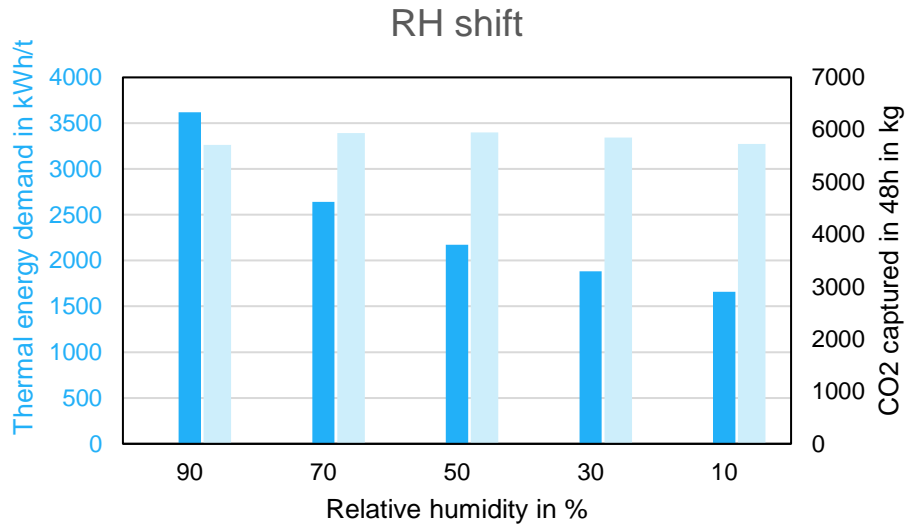
Varying the cutoff and intake concentration by varying occupancy and controlling the CO₂ level



A higher cutoff decreases the capture rate while increasing the thermal energy demand slightly

Controlling of the CO₂-level decreases capture rate and energy demand

Effect of the humidity on capture rate and energy consumption



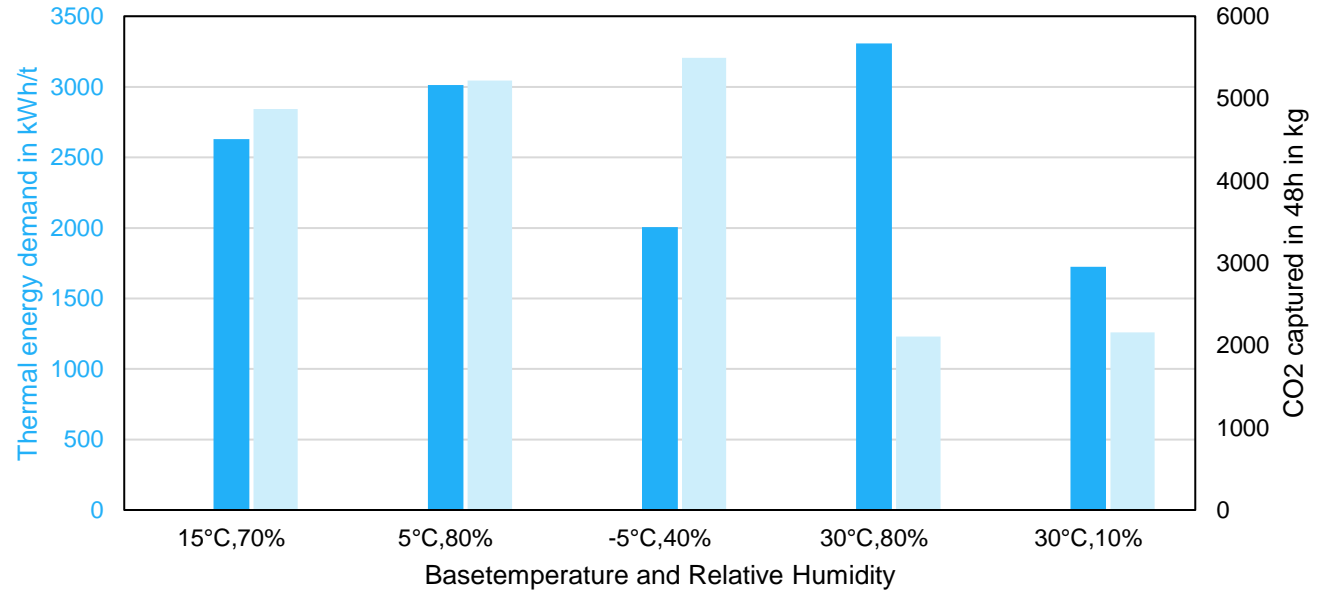
Above 70% relative humidity, water can be gained with the DAC unit, lower humidities lower the thermal energy demand

The thermal Energy demand here is calculated by the temperature difference between adsorber intake and outlet:

$$\dot{Q} = \dot{m}_{steam} \cdot c_{p,steam} \cdot \Delta T$$

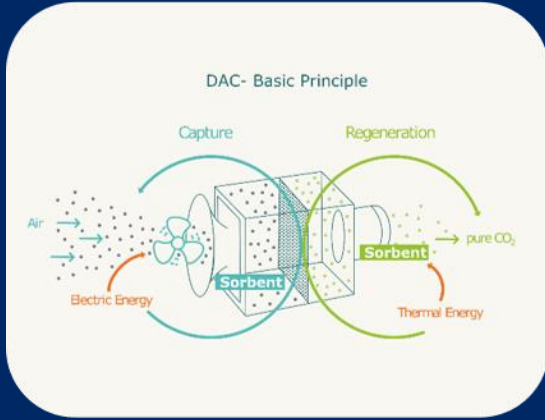
Different weather situations

Ambient temperature:
Base temperature and
increasing diurnal
variation
Cold dry conditions
proof beneficial

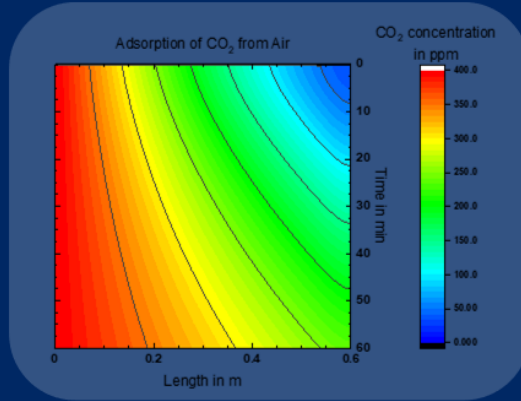


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DAC- Principles



Modelling



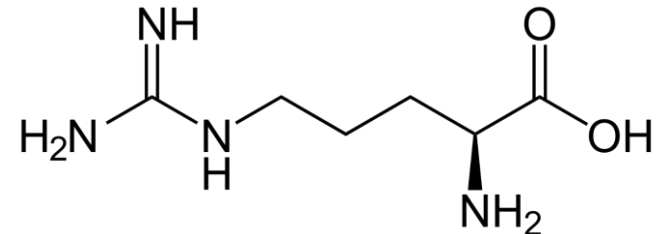
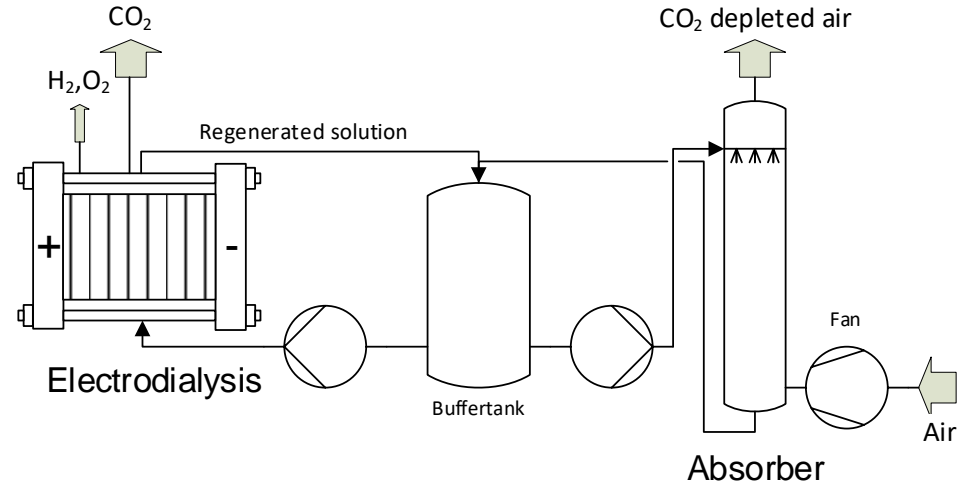
Arginine System



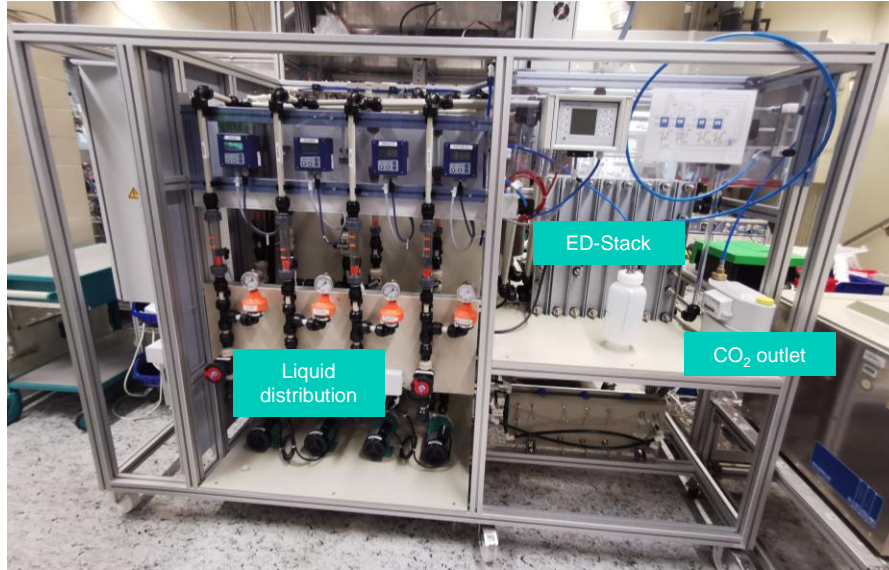
Agenda

Electro Swing Approach: Arginine Absorption

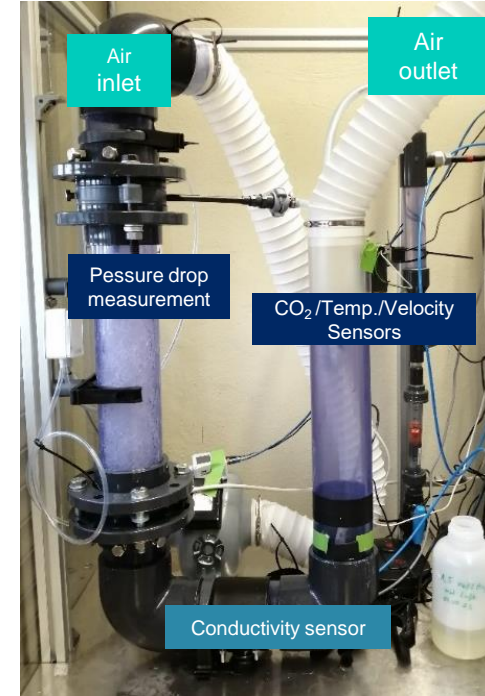
- L-Arginine is a selective chemical solvent already used for CO₂ capture from flue gases
- Arginine is sold as fitness supplement and for livestock and is therefore safe to handle
- Loaded L-Arginine can be regenerated electrochemically by electro dialysis
- Mass transport limitations due to low CO₂ concentration in air; 3D printed structures to enhance the transport at low pressure drop
- Electro dialysis provided by Deukum GmbH



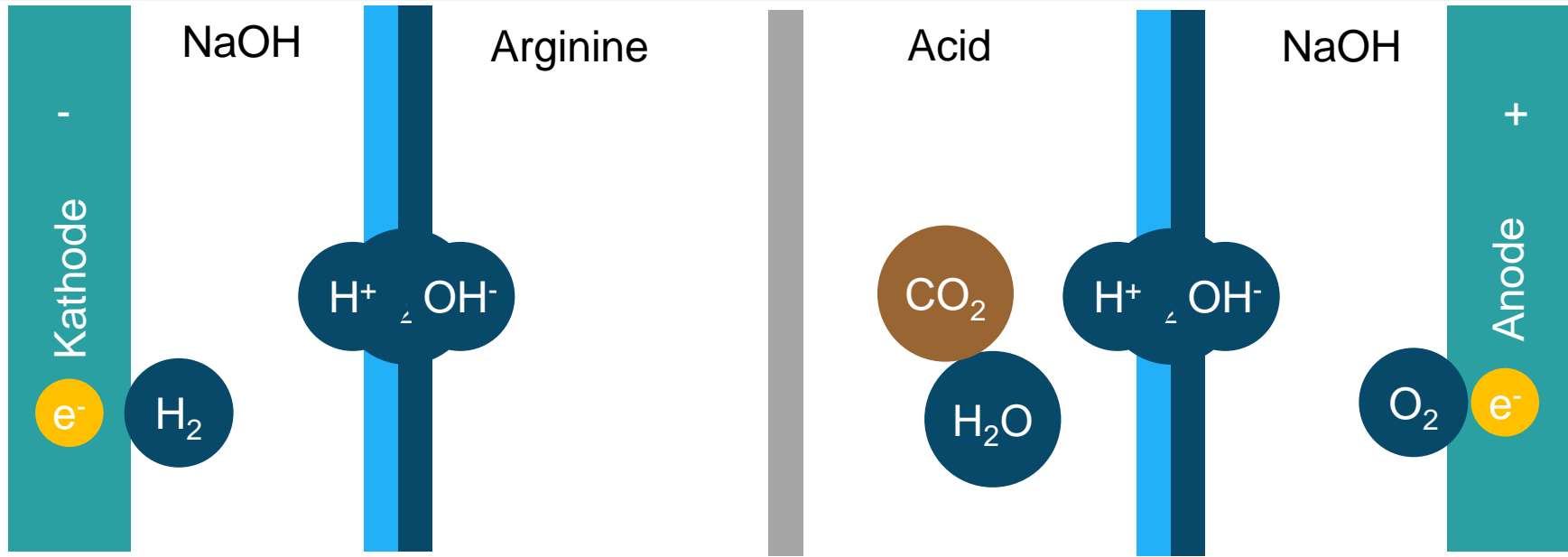
Electro Swing Approaches- L-Arginin Adsorption



The Task is to find an efficient operating window

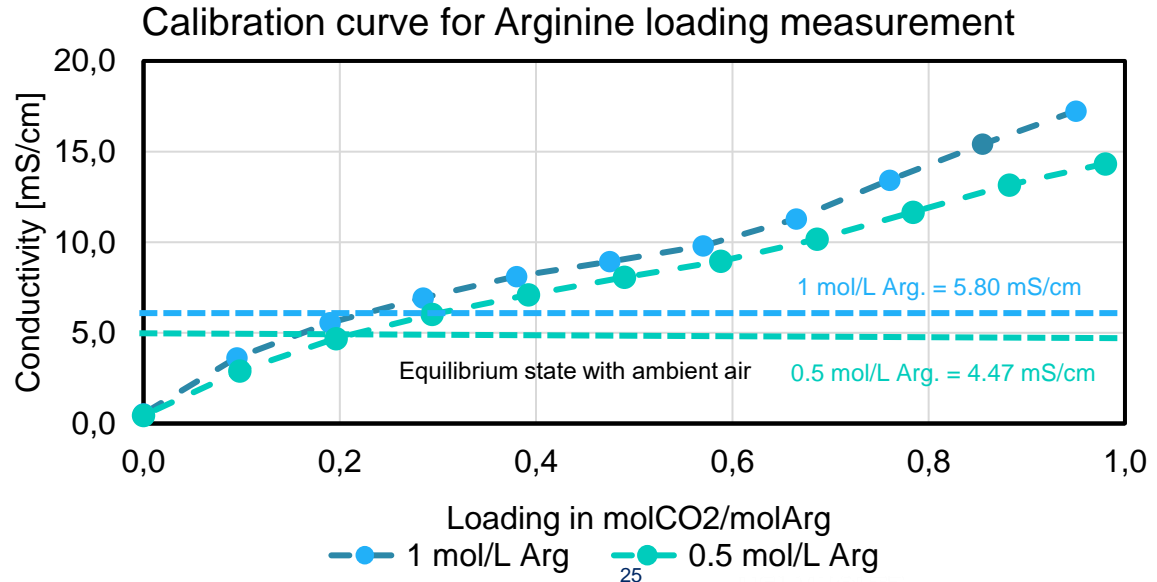
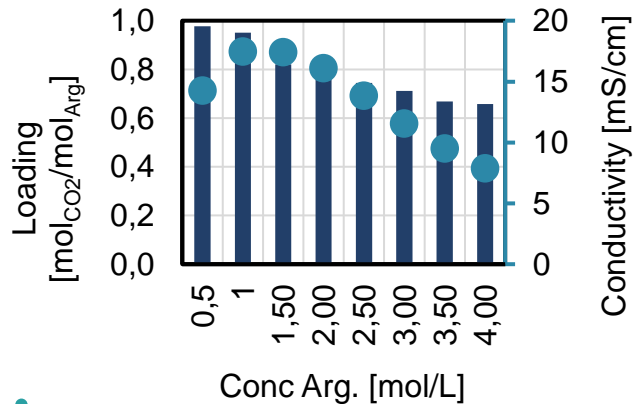


Basic Principle of Electrodialysis



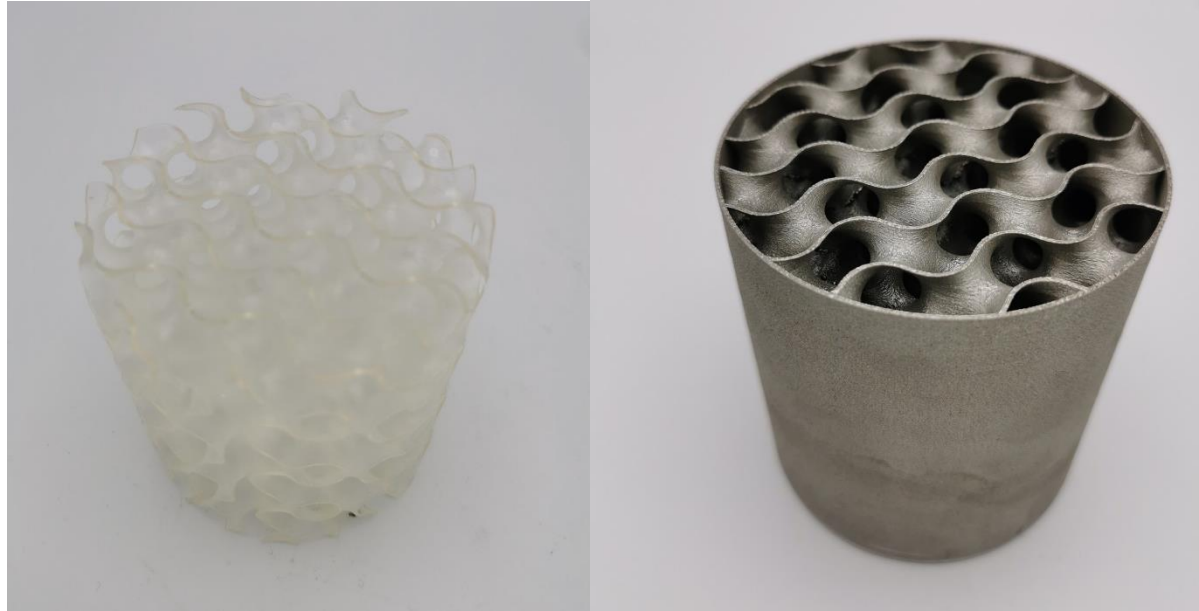
Characterization of the L-Arginin-CO₂ interaction

- First item was the quantification of the capacity of Arginine to absorb CO₂ and the calibration of the conductivity measurement
- Maximum of loading per molecule of Arginin is around one, with increasing concentration of Arginin, the relative CO₂ capacity decreases, while the absolute capacity increases
- The solubility of pure Arginin is limited to around 1 mole per liter of water. Higher concentrations must be obtained by partial CO₂ loading. The CO₂ loading then must be kept above the solubility limit



3d-printed Gyroid structures as efficient absorber packings

- Gyroids are triply periodic minimal surface bodies
- Can be additive manufactured from different materials
- Offer low pressure drop, while increasing the mass transport into the liquid
- Structurally very rigid
- Characterized by surface to volume ratio

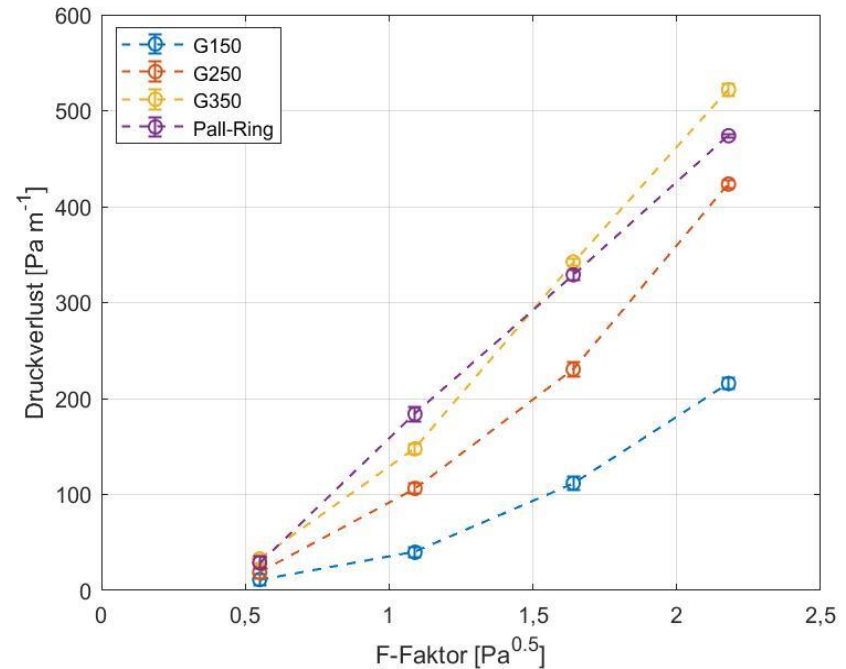


Pressure drop measurements of the different packing materials

- Pall ring packing as standard industrial solution
- Dry pressure drop:
 - Gyroids up to a surface ratio of $250 \text{ m}^2/\text{m}^3$ offer lower pressure drop
 - Similar pressure drop to the Gyroid 350 (similar surface ratio)

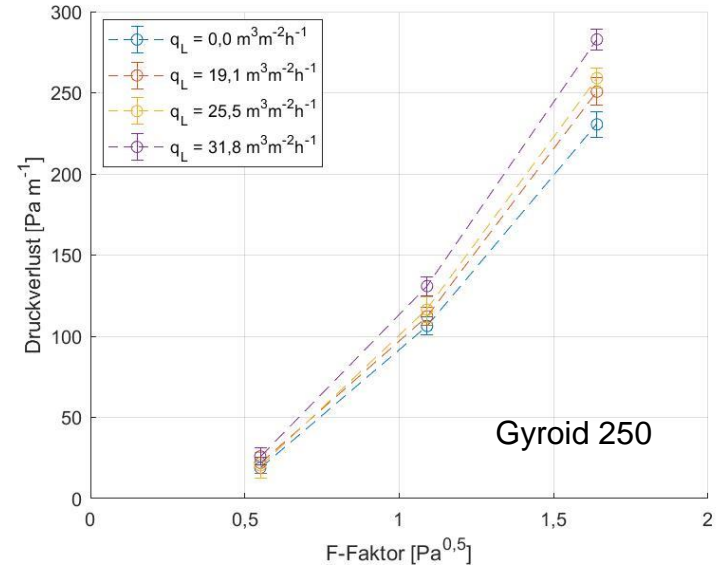
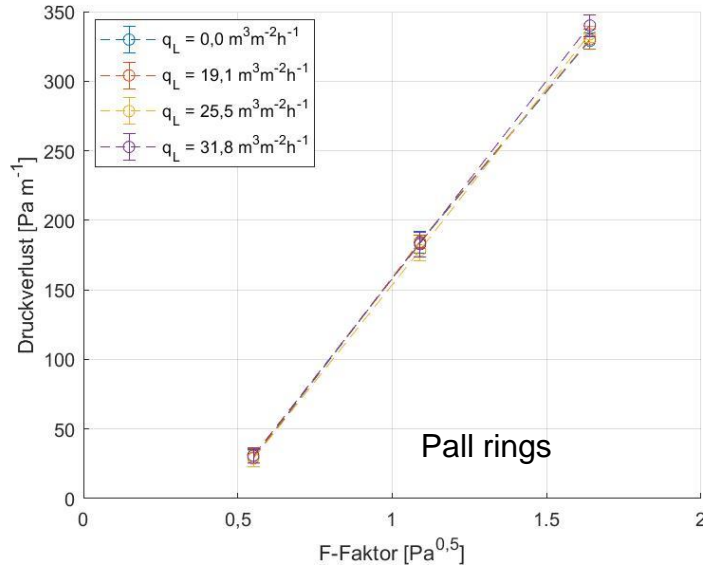


Bild: Munters



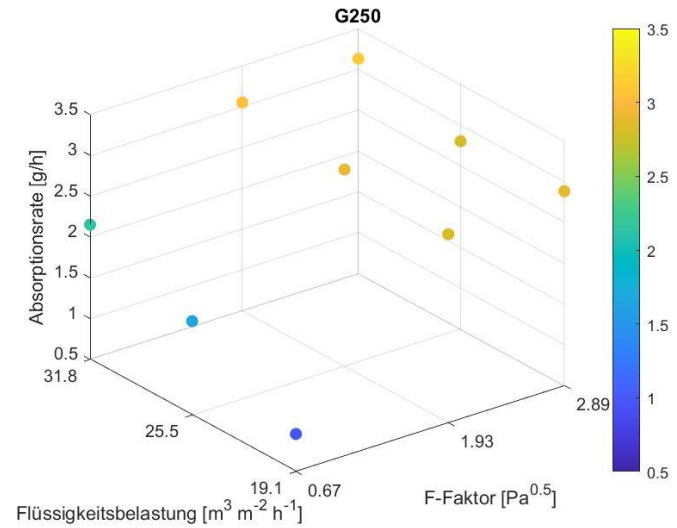
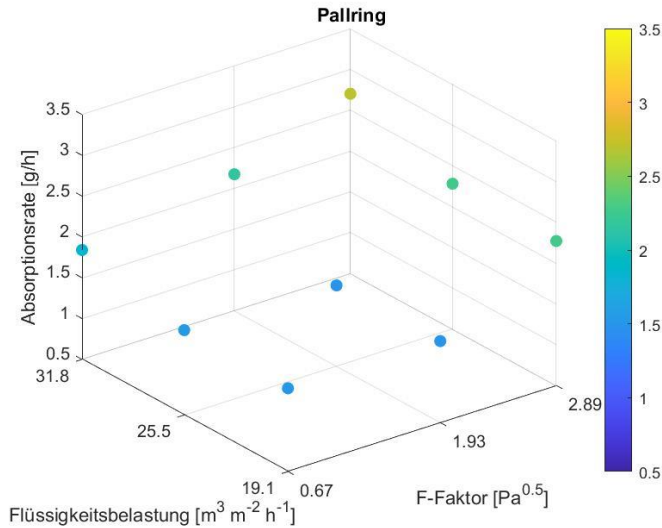
$$F = u_G \cdot \sqrt{\rho_G}$$

Wet pressure drop at varying liquid flows



$$F = u_G \cdot \sqrt{\rho_G}$$

Mass transport properties of Gyroids compared to the pall ring packing



$$F = u_G \cdot \sqrt{\rho_G}$$

Summary and outlook

- DAC will provide a necessary contribution to a cyclic carbon economy and negative emissions
- The integration into existing ventilation systems can have certain benefits, if the plant is controlled smart
- L-Arginine proves to be a viable alternative technology in the future
- The liquid adsorbent must be scaled up and directly linked to the Electrodialysis
- The rooftop lab has to provide real world data

Thanks a lot for your attention!



This work was performed as part of the project 'A Comprehensive Approach to Harnessing the Innovation Potential of Direct Air Capture and Storage for Reaching CO_2 -Neutrality' (DACStorE), which is funded by the Initiative and Networking Fund of the Helmholtz Association (grant agreement number KA2-HSC-12).