DYNAMIC WATER SORPTION - EXPERIMENTS AND LESSONS LEARNED

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Fraunhofer Institute for Solar Energy Systems ISE

Leipziger Symposium on dynamic sorption

Leipzig, 17th April 2018

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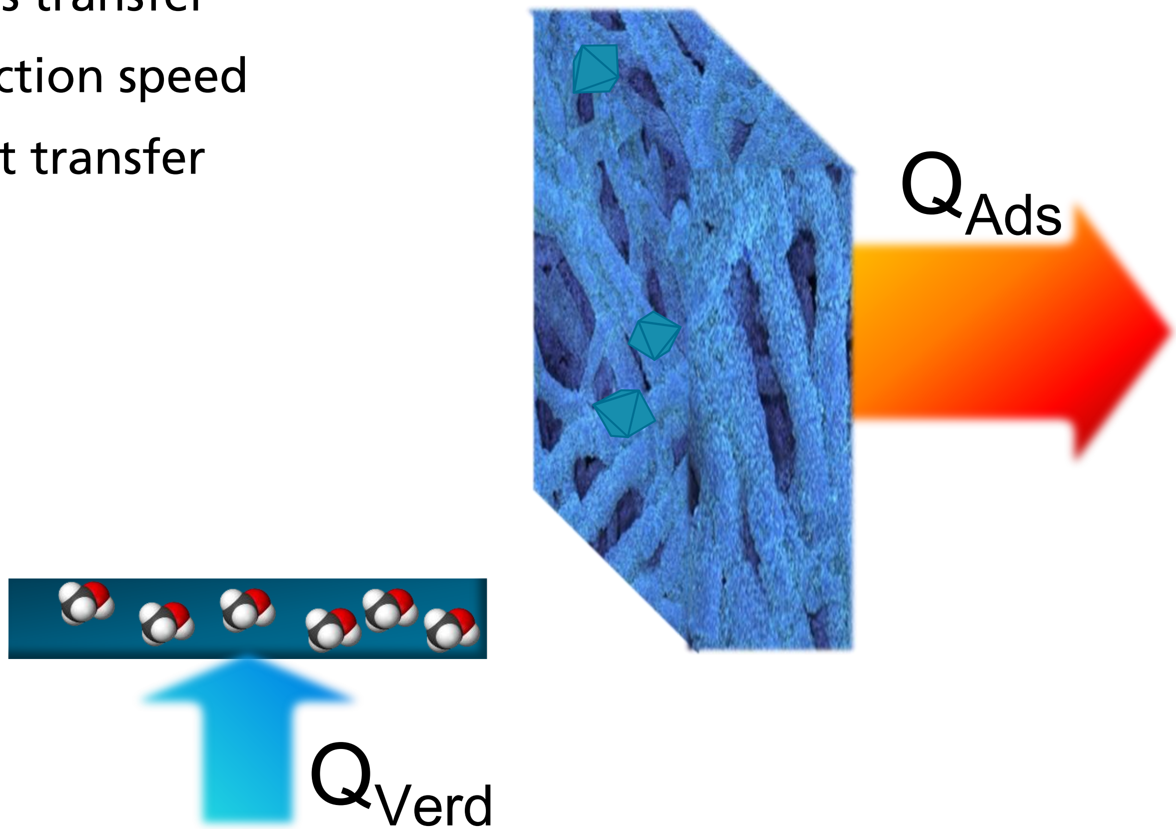
AGENDA

- Motivation
- Closed applications / pure gas
  - Large Pressure Jumps (LPJ) MeOH/AC Rubotherm TG
  - Large Temperature Jump (LTJ) in kinetic setup
  - Large Pressure Jump (LPJ) in kinetic setup
  - Frequency Response
- Open applications / gas mixtures
  - Dehumidification of (process) air
- Conclusion

Motivation

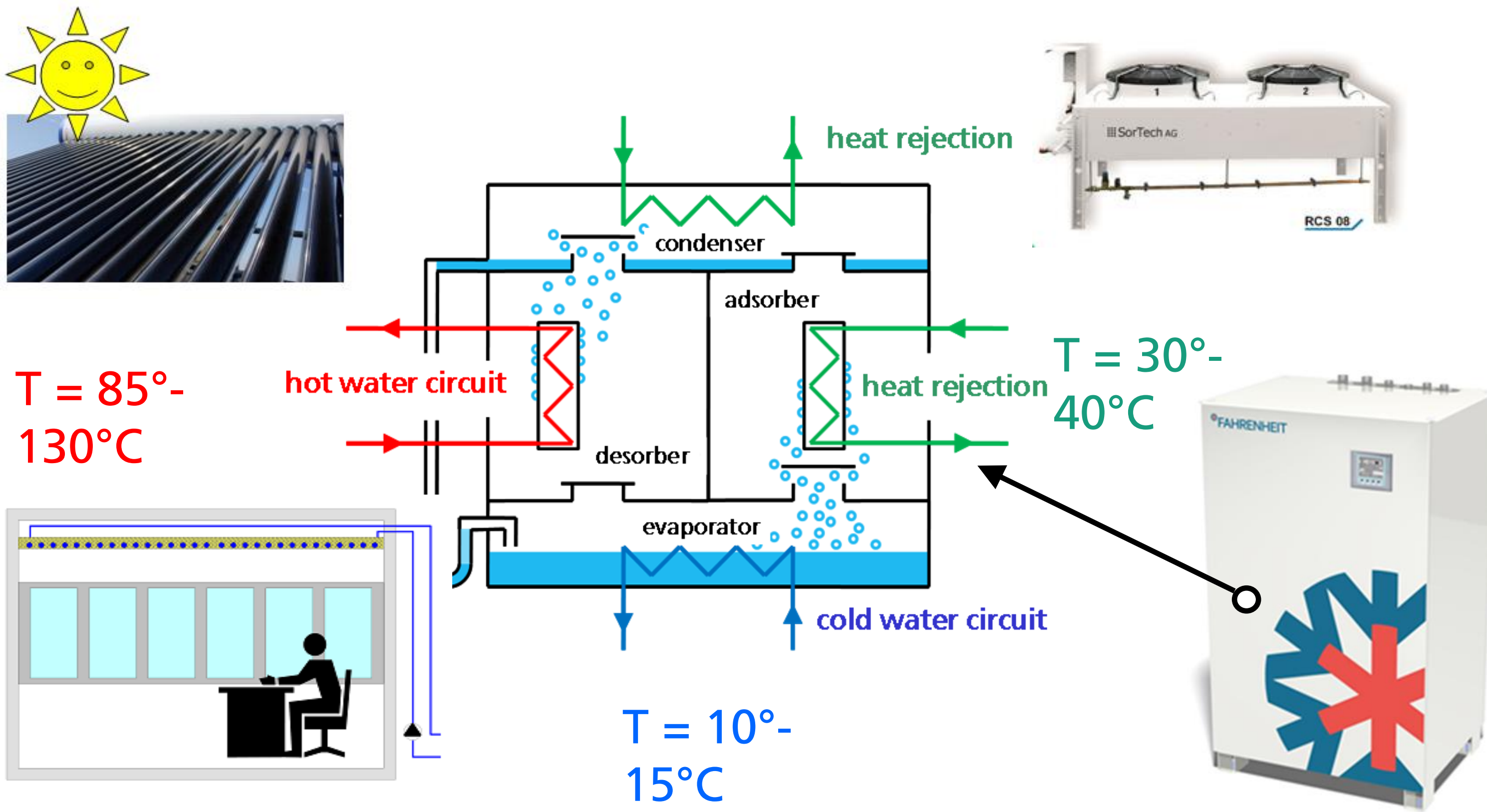
- Dynamics depend on different processes
  - Mass transfer
  - Reaction speed
  - Heat transfer



Motivation

- Application in focus:

  Adsorption heat pumps and chillers ➔ Dynamics = power (density)



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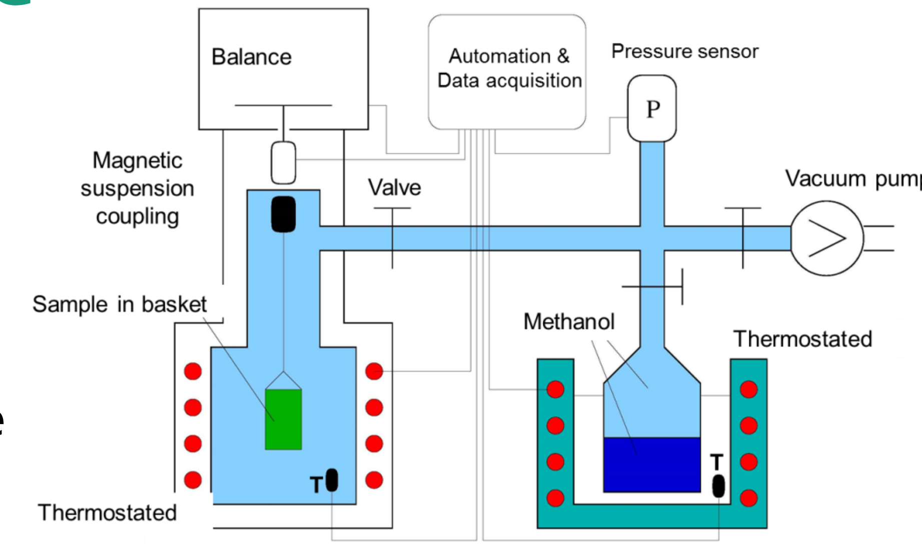
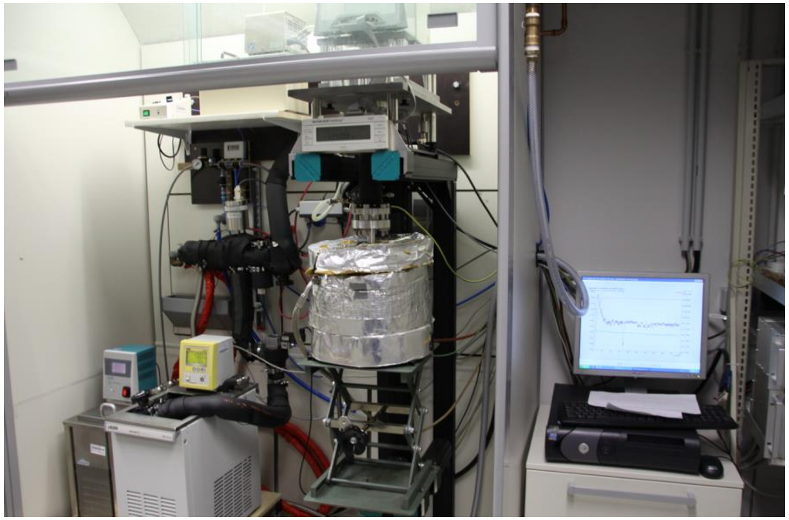
Closed / pure gas
LPJ MeOH/AC Rubotherm TG

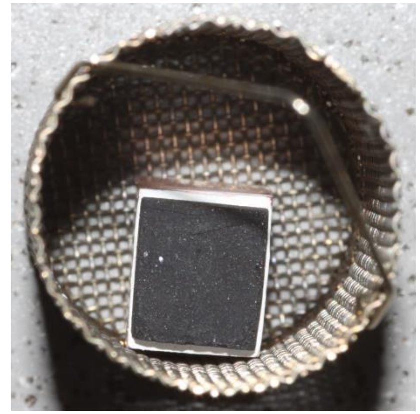
- Characterization of Activated Carbon extrudate
- Pretreatment / regeneration of the sample
- Pressure Jump after opening a valve
- Detection of uptake (balance)



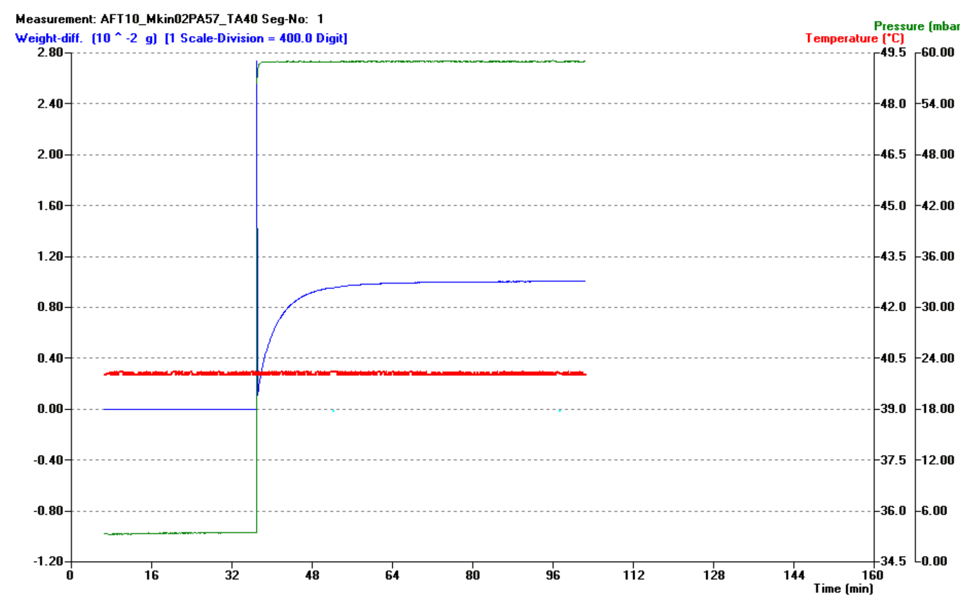


Closed / pure gas

LPJ MeOH/AC Rubotherm TG



- Characterization of Activated Carbon extrudates
- Results (fitting to model):
  - D_{eff} = 2-8 * 10^{-5} m²/s
- Challenge:
  - Keep the adsorbent in isothermal condition
  - No detection of sample temperature ➔ missing information!



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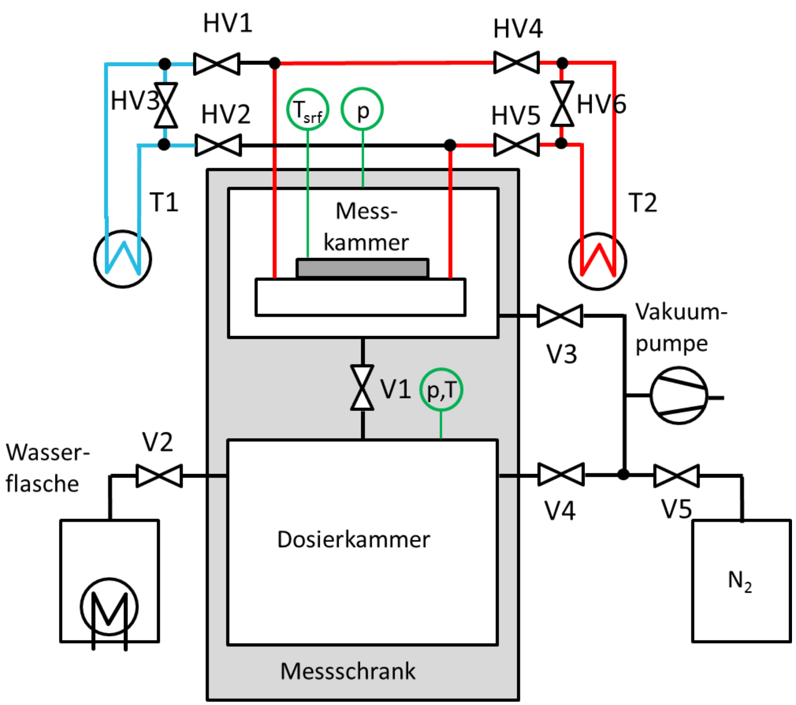
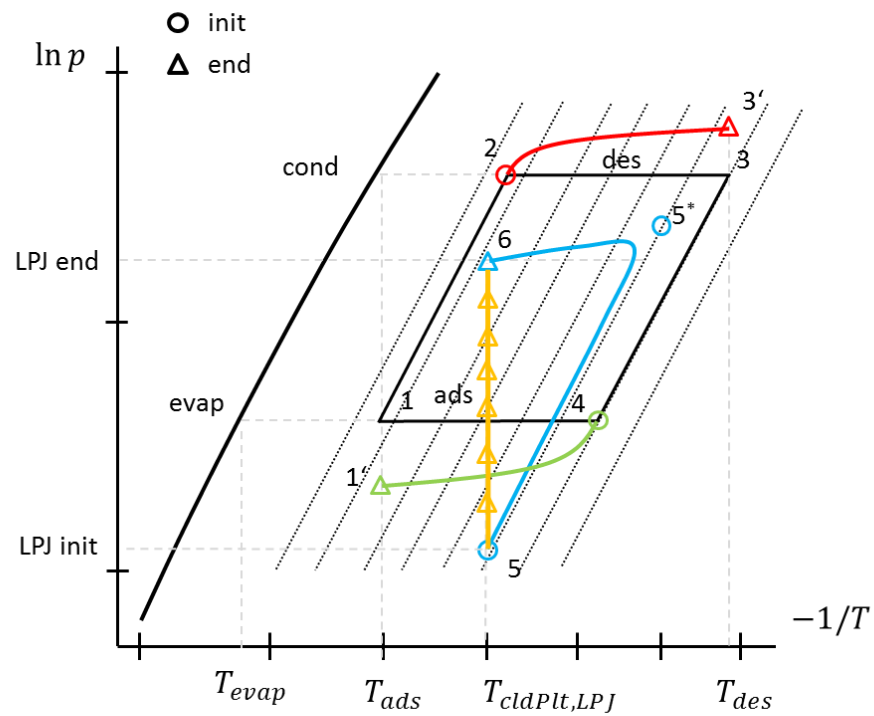
Closed / pure gas
Kinetic setup at Fraunhofer ISE





- Large Pressure Jump (LPJ), Large Temperature Jump (LTJ), inert-LTJ, and Small Pressure Jumps (SPJ) are „Standard“methods

Velte, PhD Manuscript 2018

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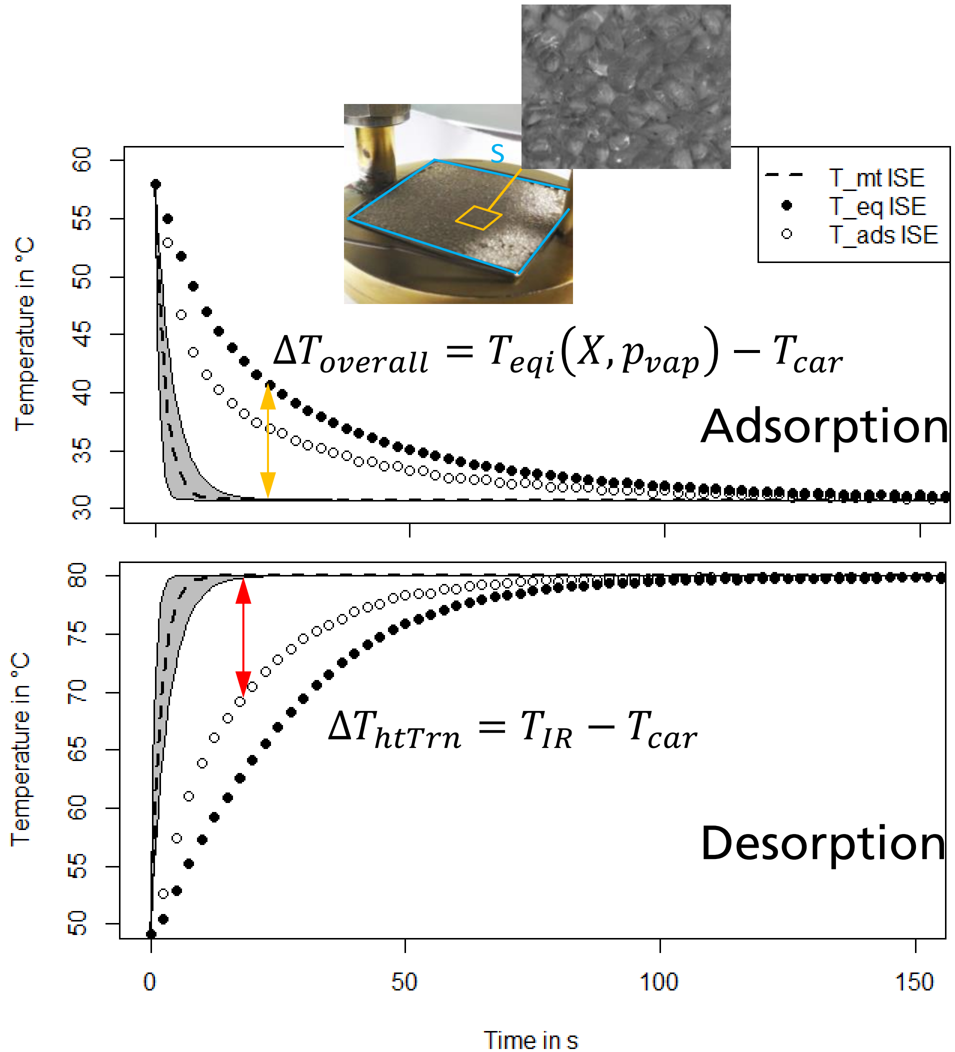
LAUDA
Julabo

Closed / pure gas

LTJ - Driving temperature differences

- Here: LTJ data for adsorption and desorption of Silicagel (Ø0.9 mm)
- Simple numerical model: Equilibrium data to calculate T_{eqi}
- Temperature difference for heat transfer ΔT_{htTrn} and overall driving temperature difference $\Delta T_{overall}$
- If $\Delta T_{htTrn} \approx \Delta T_{overall}$: Strong heat transfer limitation
- If $\Delta T_{htTrn} \ll \Delta T_{overall}$: Strong mass transfer limitation

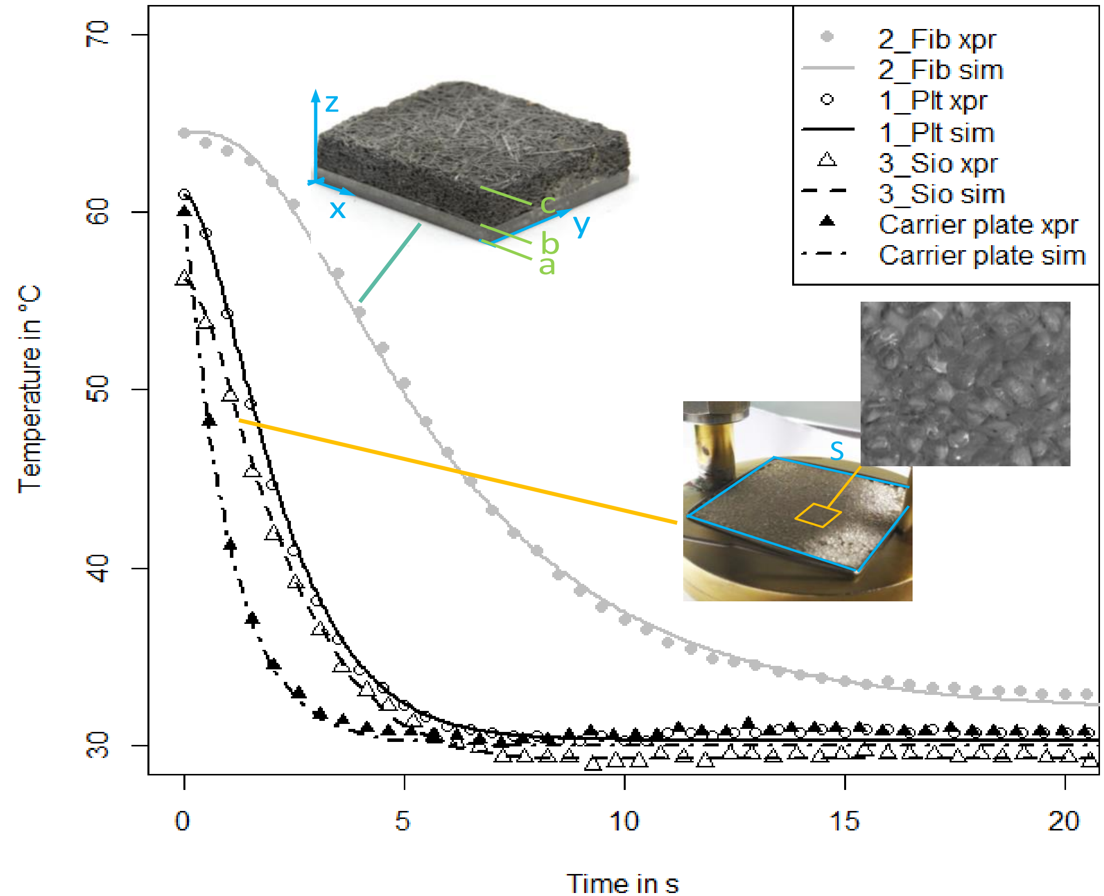


Velte, PhD Manuscript 2018

Closed / pure gas

LTJ, evaluation of Heat transfer in inert gas

- Here: LTJ data under N_2 atmosphere
- No sorption during temperature jump
- Identification of heat transfer parameters without influence of sorption effects

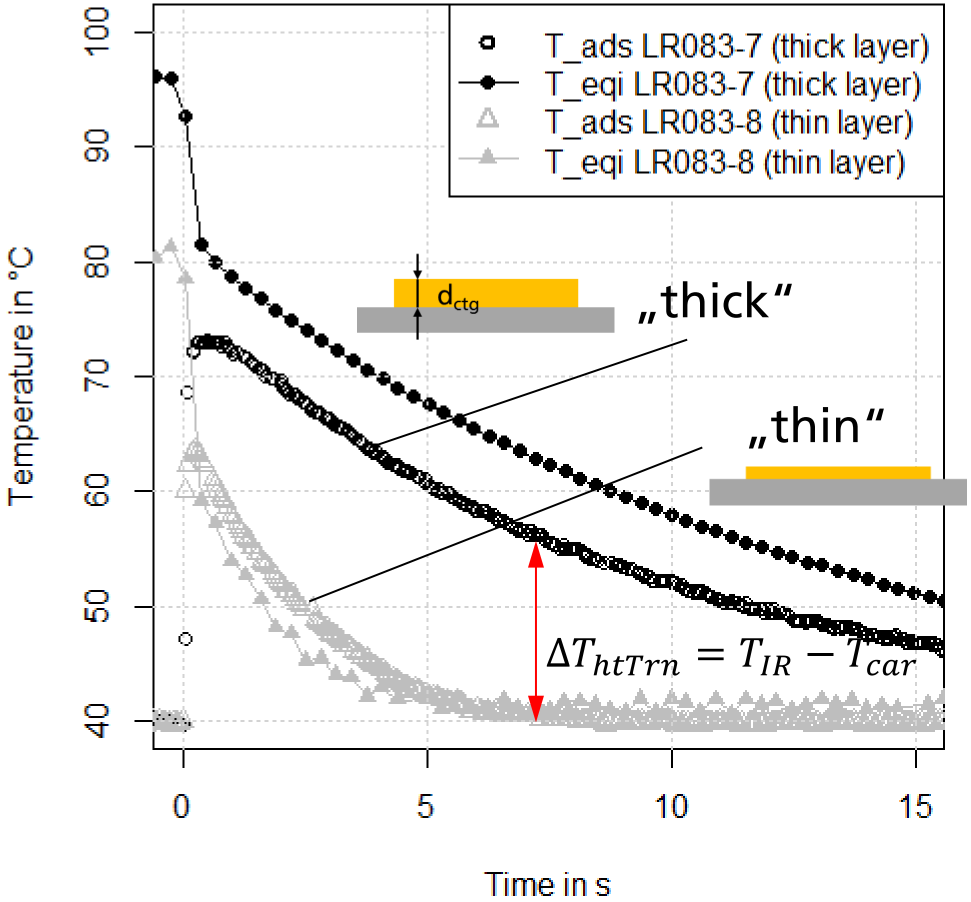


Velte et al., (submitted), Energies, 2017

Closed / pure gas

LPJ - Driving temperature differences

- Here: LPJ data for two samples with a binder based NaY coating (Spray coating)
- Both samples show a strong heat transfer limitation
- But: Adsorption kinetics are very fast
- For the „thick“ sample ($d_{ctg} \approx 450\ \mu m$) mass transfer begins to play a role

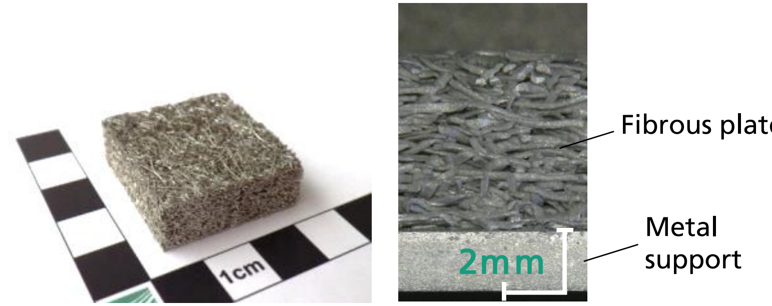


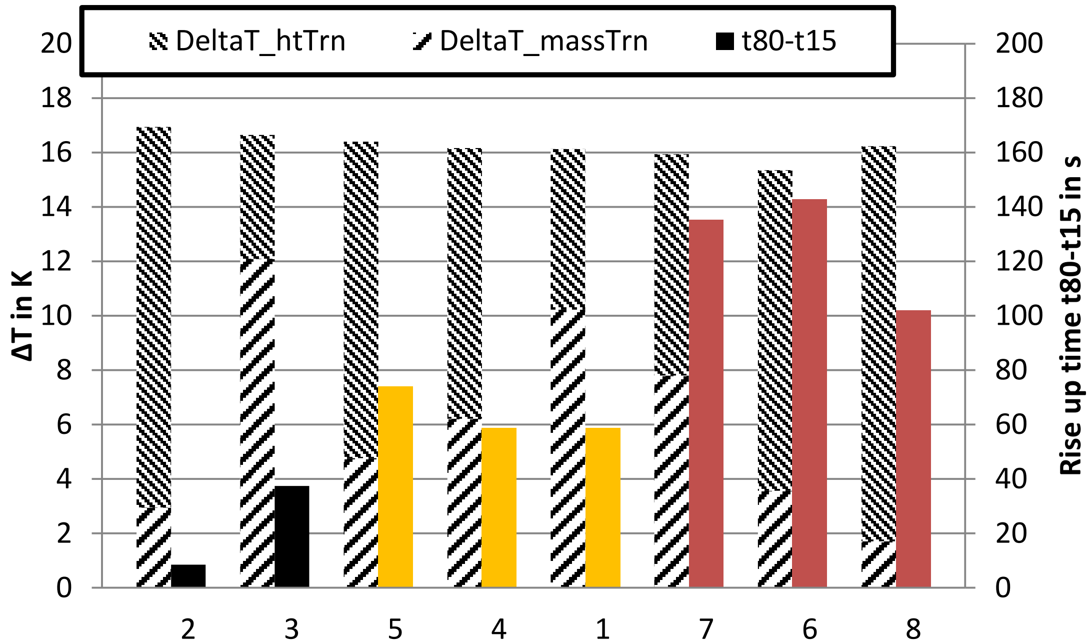
Velte, PhD Manuscript 2018

Closed / pure gas

Identifying heat and mass transfer resistances

- Is it always the heat transfer?
- For different directly crystallized samples (crystallite layer thickness $d_{cryst} = 14 \dots 30\ \mu m$) both heat and mass transfer play a role
- Results can help to build optimized heat exchangers





$d_{cryst} =$	14	18	22	23	24	24	26	27
$d_{maP} =$	625	195	343	360	214	119	151	457
$d_{cmp} =$	3.0	2.9	2.9	2.8	2.9	5.0	5.0	5.7

[6] Velte et al., Heat Powered Cycles Conf. 2016

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LPJ / LTJ – Modelling: Non-isothermal ads. kinetics (PDE)

Mass balance

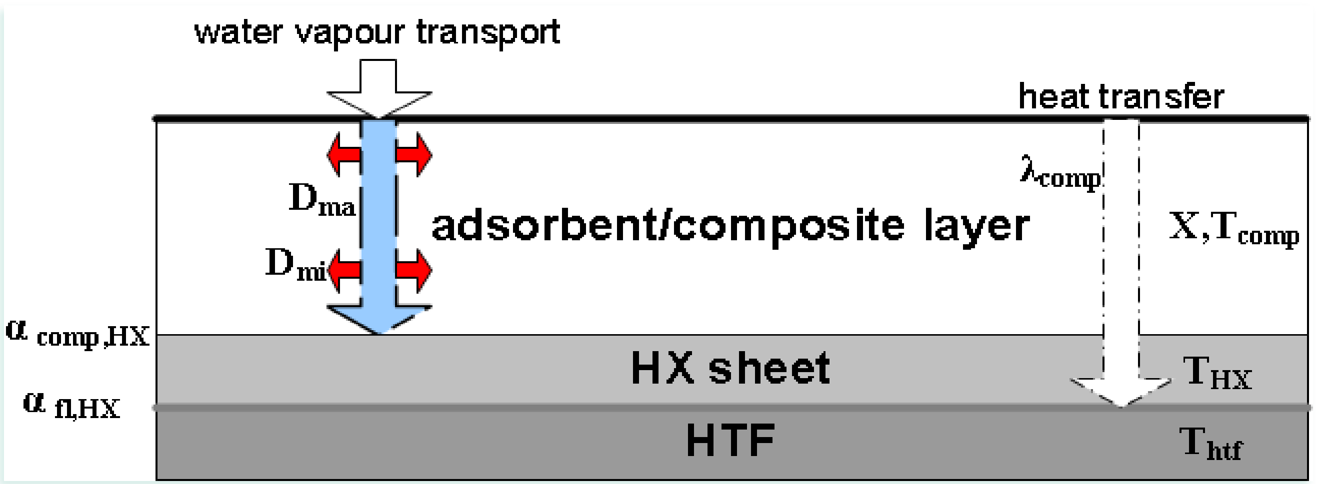
$$\frac{\partial c_g}{\partial t} = \frac{\partial}{\partial x}\left(D_{ma}\frac{\partial c_g}{\partial x}\right) + \frac{\dot{n}}{A_{mi}}\frac{4\psi_{mi}}{d_{ma}}$$

$$\frac{\partial c_g}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD_{mi}\frac{c_{ad}}{c_g}\frac{\partial c_g}{\partial r}\right) - \frac{\rho_{crys}^{dry}}{M\,\psi_{mi}}\frac{\partial X}{\partial t}$$

Heat balance

$$\rho_{comp}^{dry} c_p^{comp}\frac{\partial T_{comp}}{\partial t} = \frac{\partial}{\partial x}\left(\lambda_{comp}\frac{\partial T_{comp}}{\partial x}\right) + h_{ad}\rho_{comp}^{dry}\zeta_{ad}\frac{\partial X}{\partial t}$$

$$h_{ad} = h_{ev} + A$$



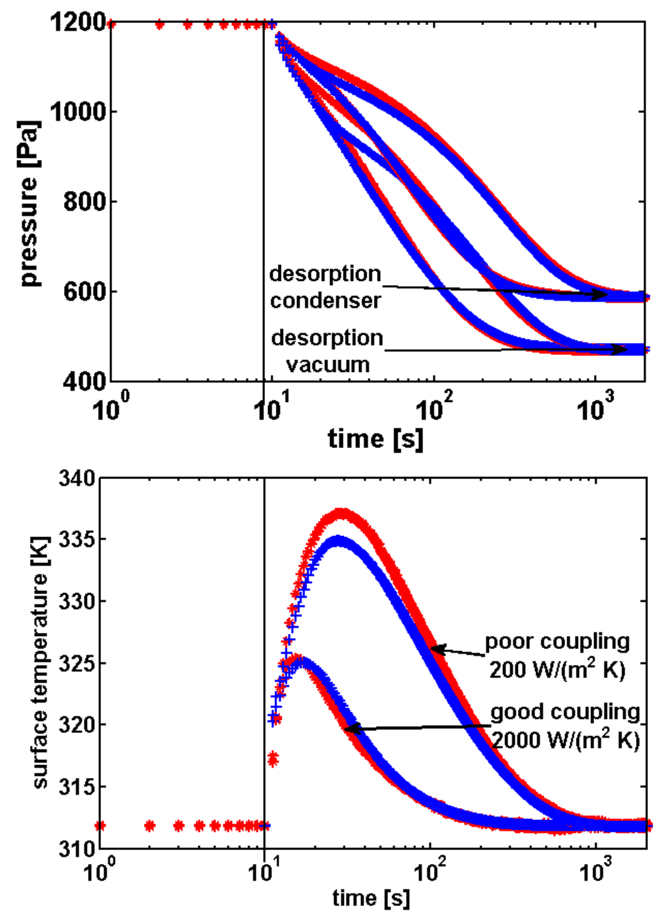
Füldner 2015, PHD thesis, 10.6094/UNIFR/10072

Closed / pure gas

LPJ / LTJ – Modelling: Non-isothermal ads. Kinetics (PDE)

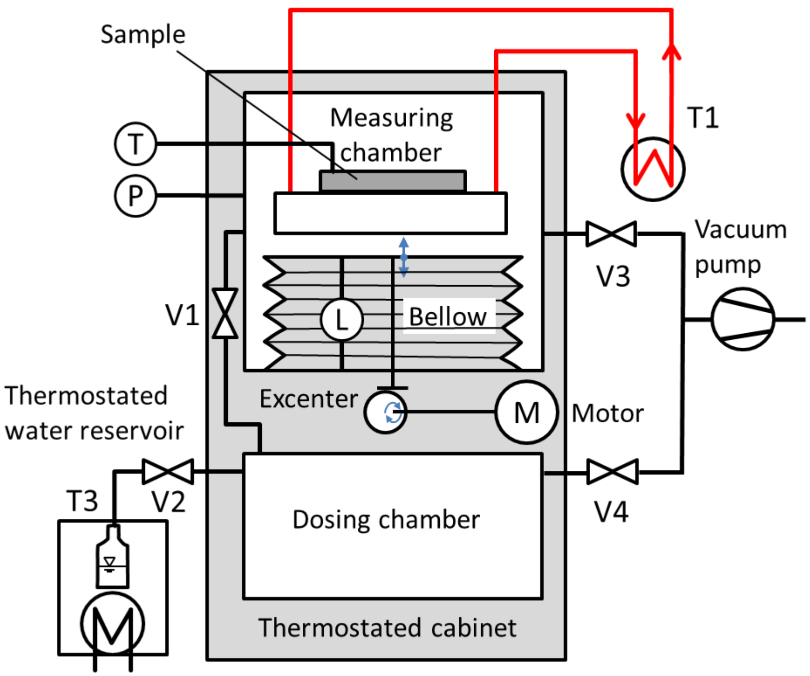
Determination of adsorption kinetics parameters

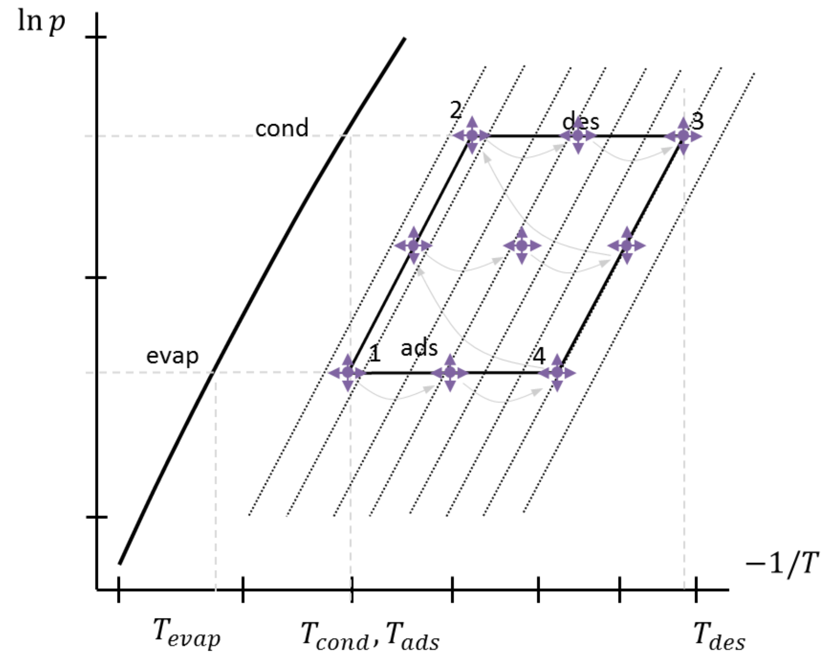
- Experimental values (pressure p(t), temperature T(t), heat flux Q(t)) are used to parametrize:
  - Diffusion coefficient
  - thermal conductivity
  - heat transfer coefficients
- Mathematical model of the adsorption process in COMSOL Multiphysics (FEM)
- Diffusion can be described by monodisperse or bidisperse models



Füldner 2015, PHD thesis, 10.6094/UNIFR/10072

Closed / pure gas
Frequency Response Method





- Volume Swing Frequency Response (FR) measurements for in depth investigations of heat and mass as a function of pressure, temperature or loading by model fit [1] in frequency domain.

Wang, LeVan, AIChE Journal 2011, 10.1002/aic.12420.

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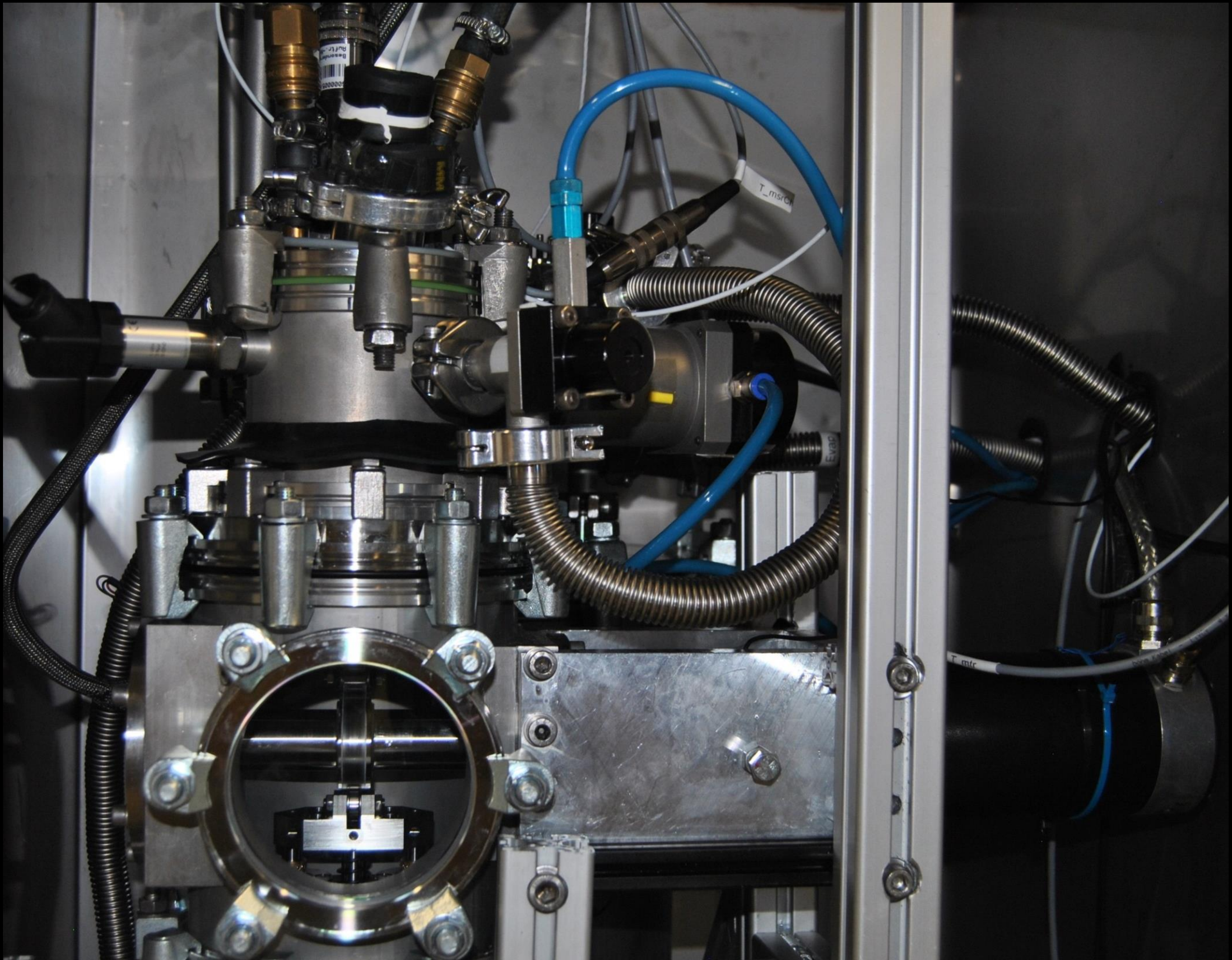
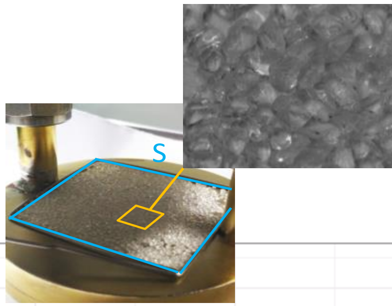

T_msrC
Evac
T_mfr

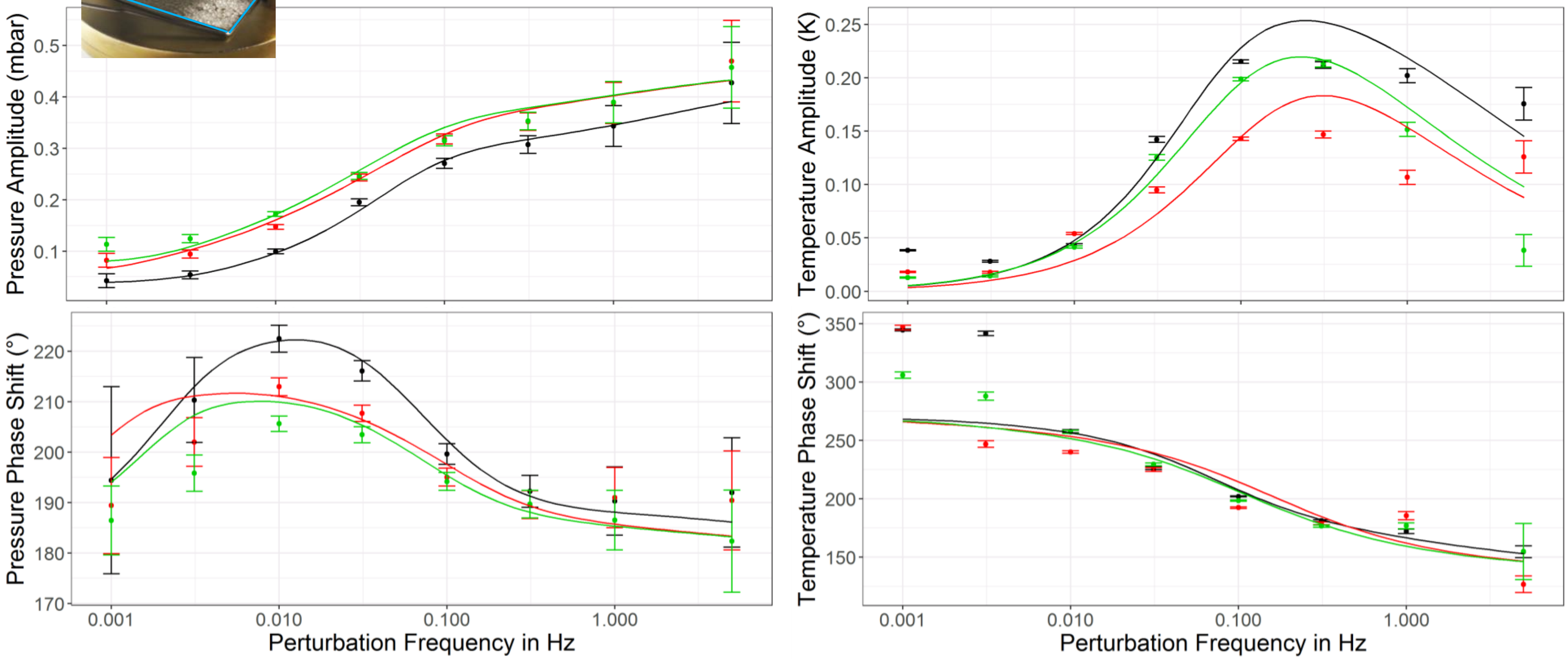
Closed / pure gas
Frequency Response Method

Tab.: Identified coefficients at11 mbar

$$k_{\mathrm{LDF}}=15\frac{D}{r2}$$

Temperature	a (W/m²K)	D (10^{-9} m²/s)
31 °C	230	6
43 °C	280	2
54 °C	220	3
31-54 °C [1]	270	5





[1] Velte et al., Energies, 2017

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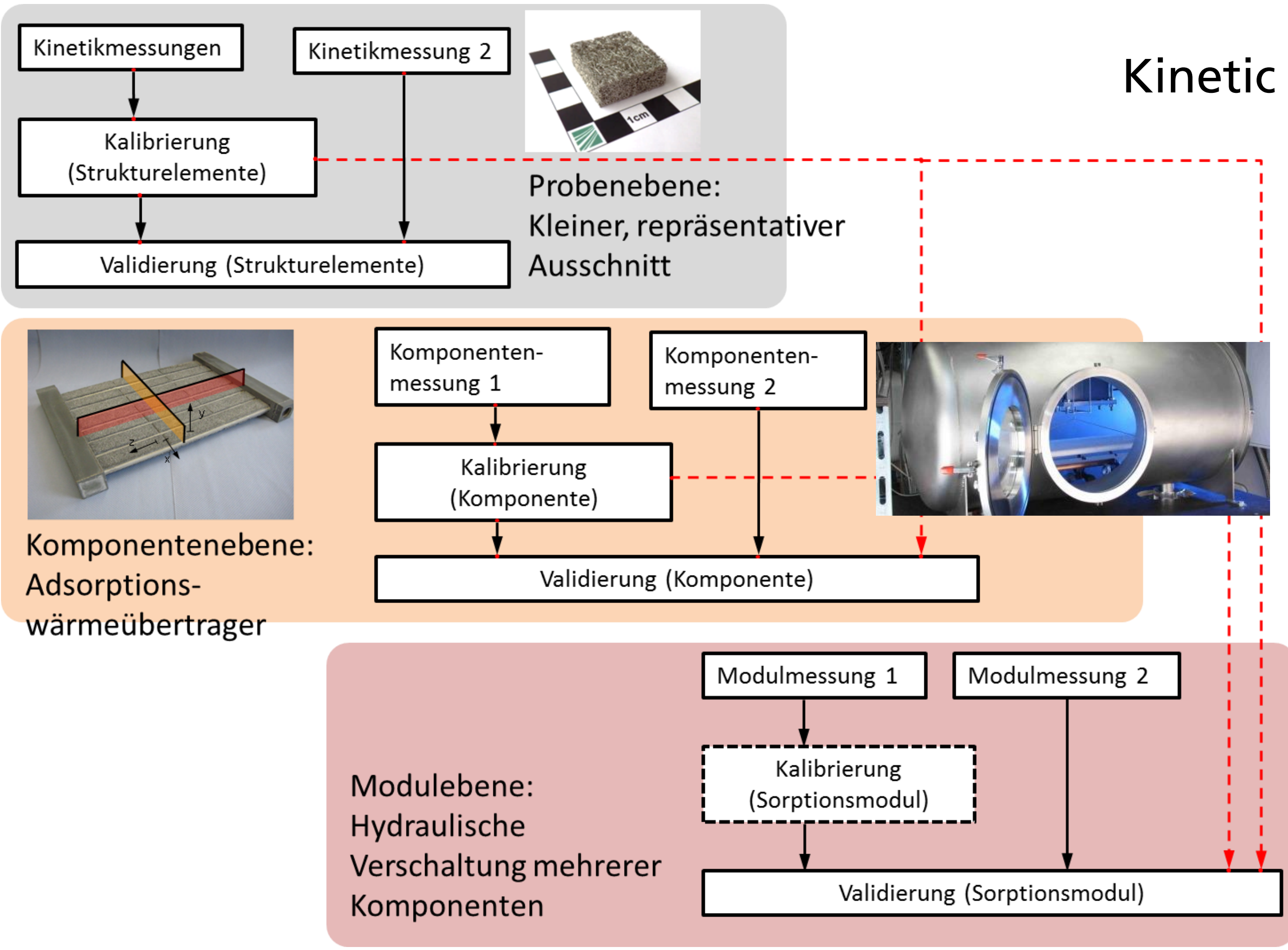
Dynamic measurements on different scales



Kinetic set-up

Adsorber level

Sorption module level

Wittstadt, Füldner et al., 10.1016/j.renene.2016.08.061
Velte, PhD Manuscript 2018

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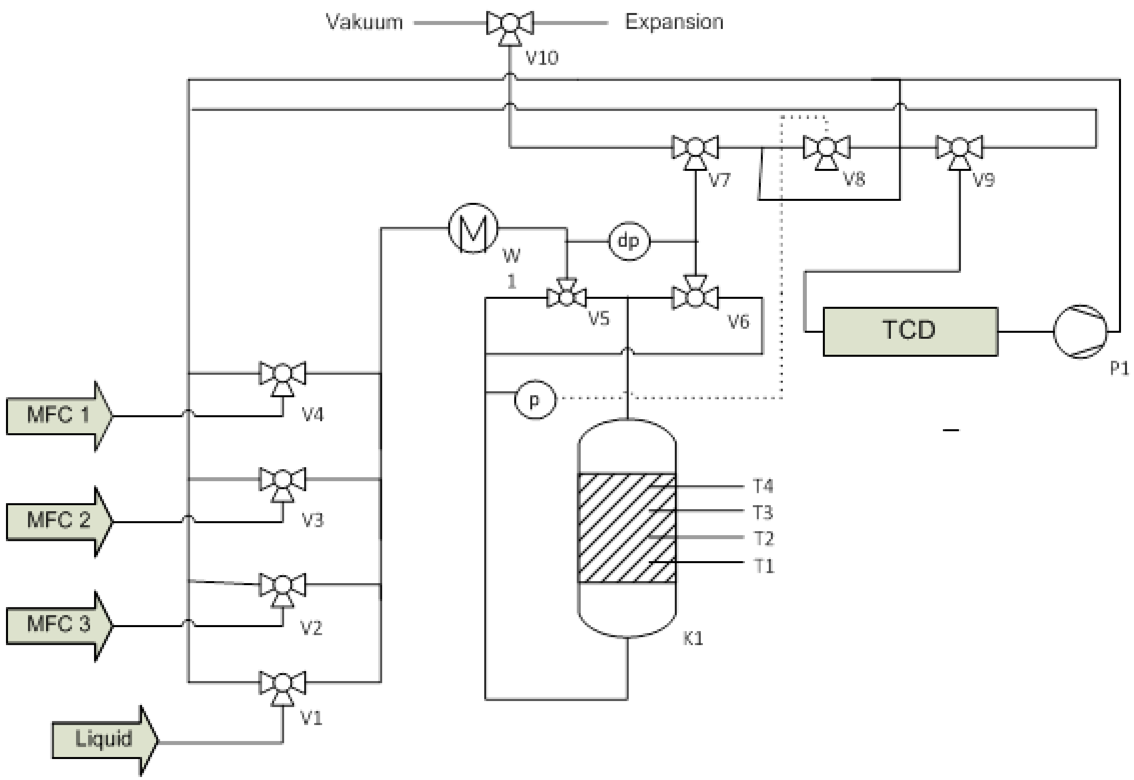
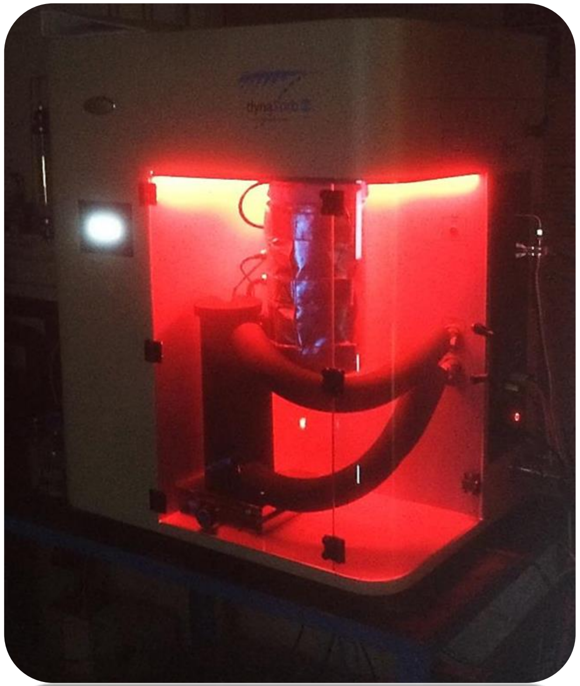
Open applications / gas mixtures
Case Studies

- Dehumidification of (process) air

Open applications / gas mixtures
Quantachrome DynaSorb BT





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Open applications / gas mixtures
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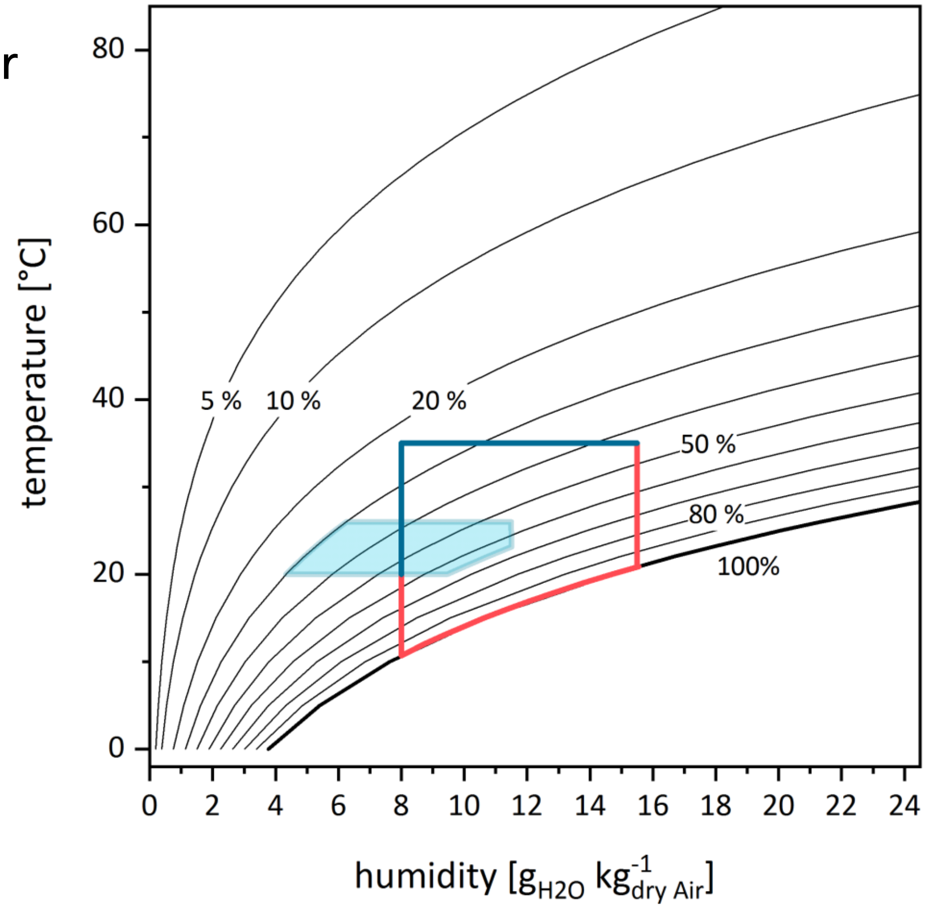

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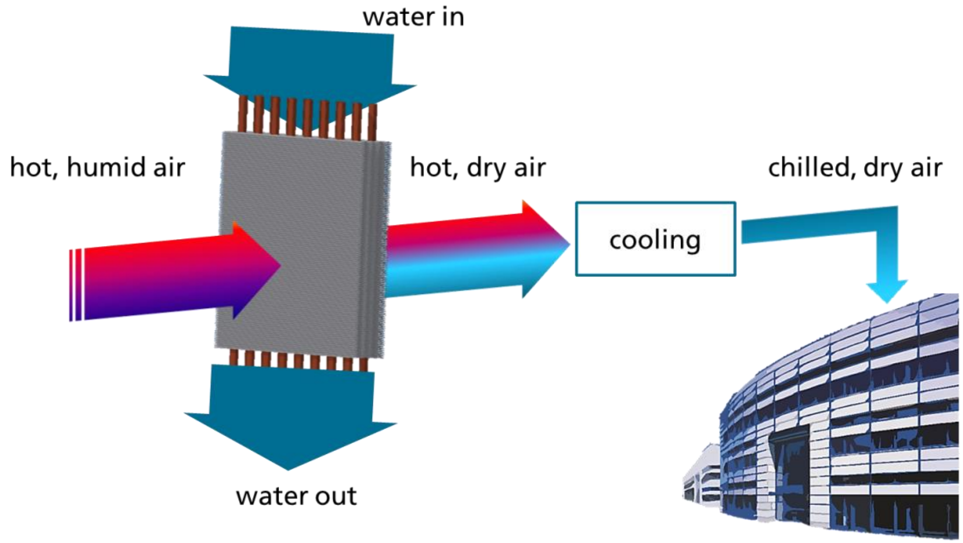

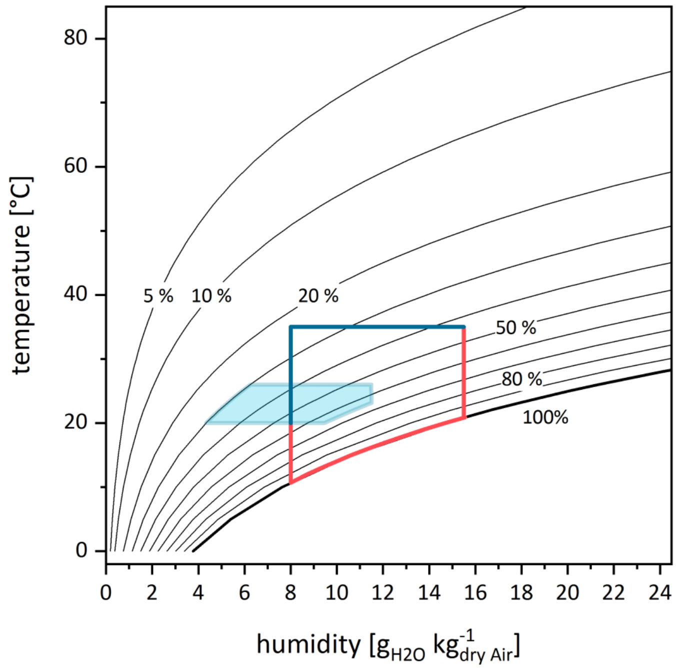

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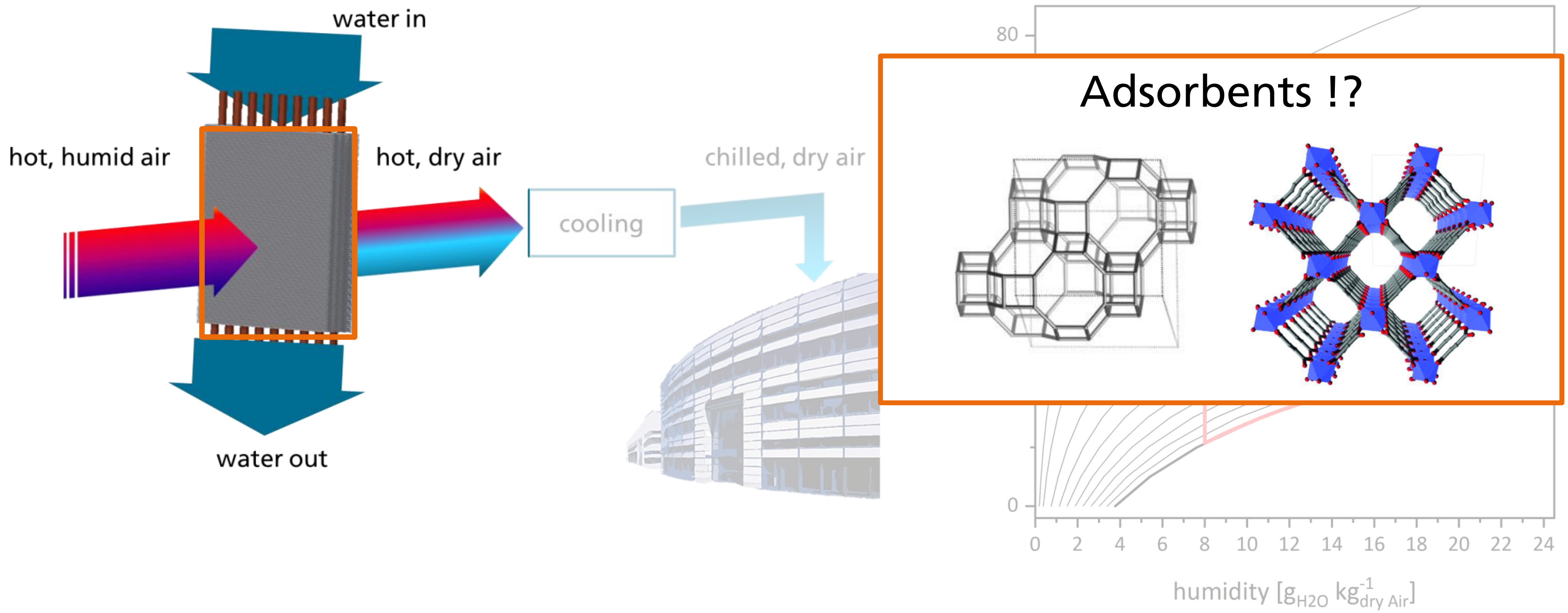

iza-structure.org, Alvarez et al (2015)

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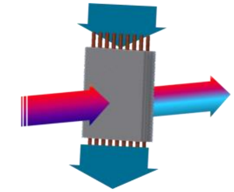
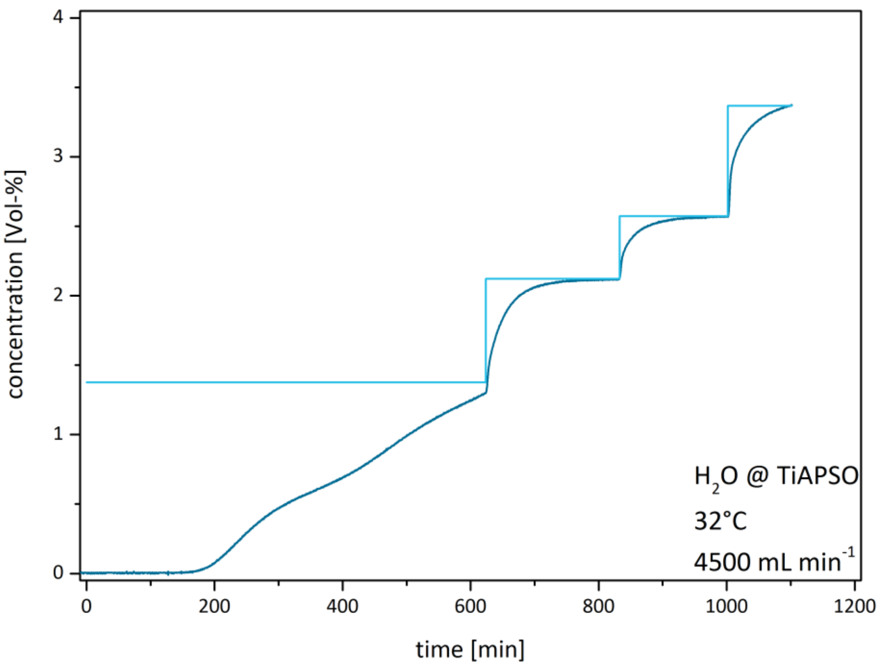
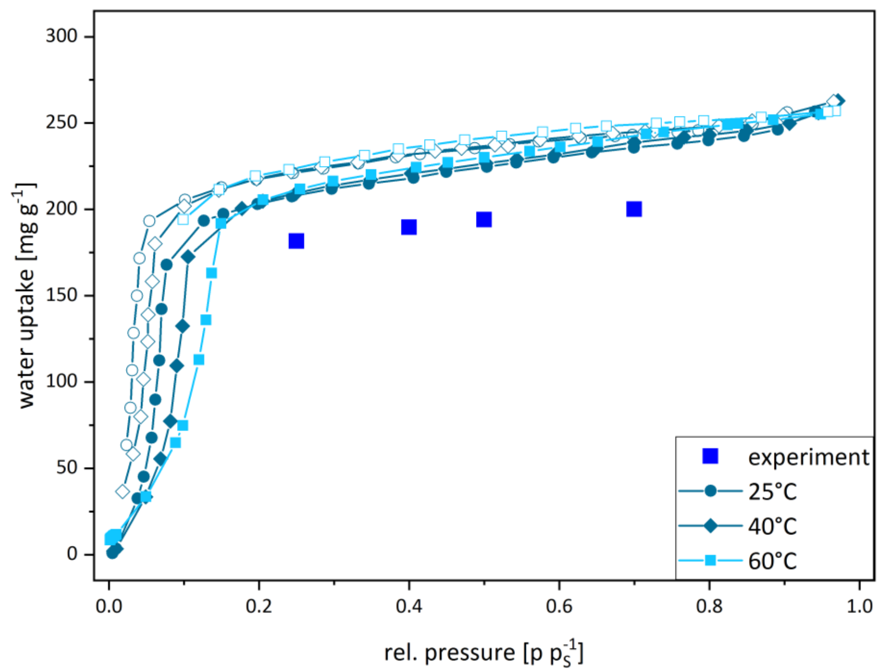
Open applications / gas mixtures
H_2O @ TiAPSO







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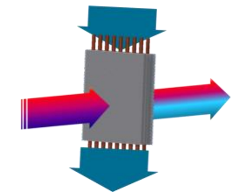
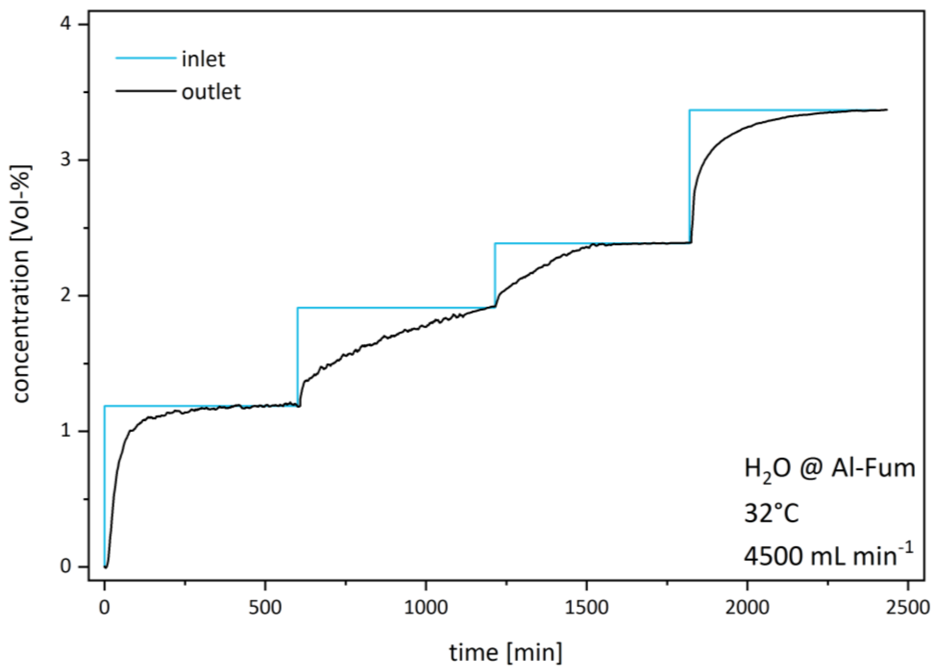
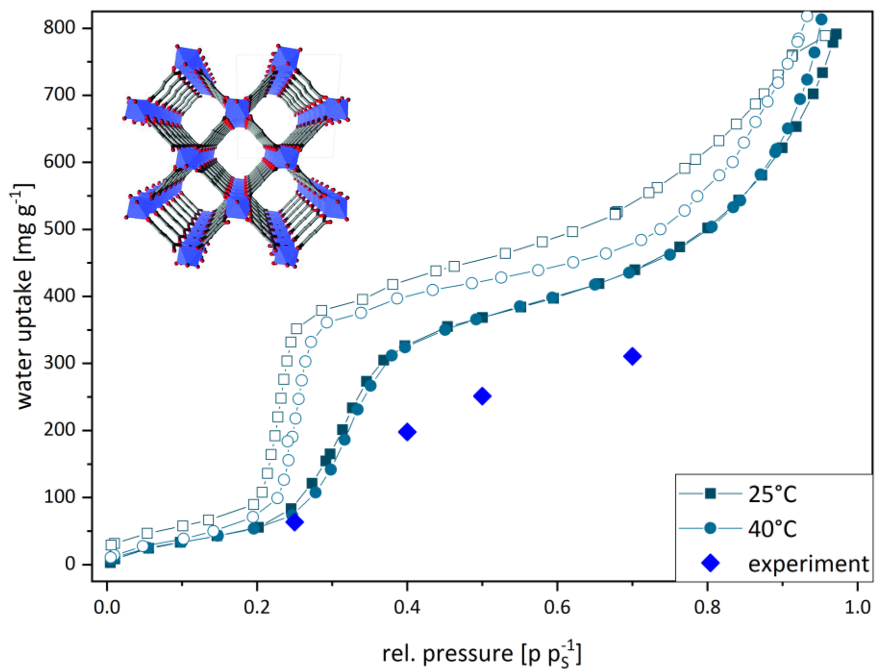
Open applications / gas mixtures

H_2O @ Al-Fumarate







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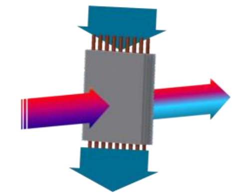
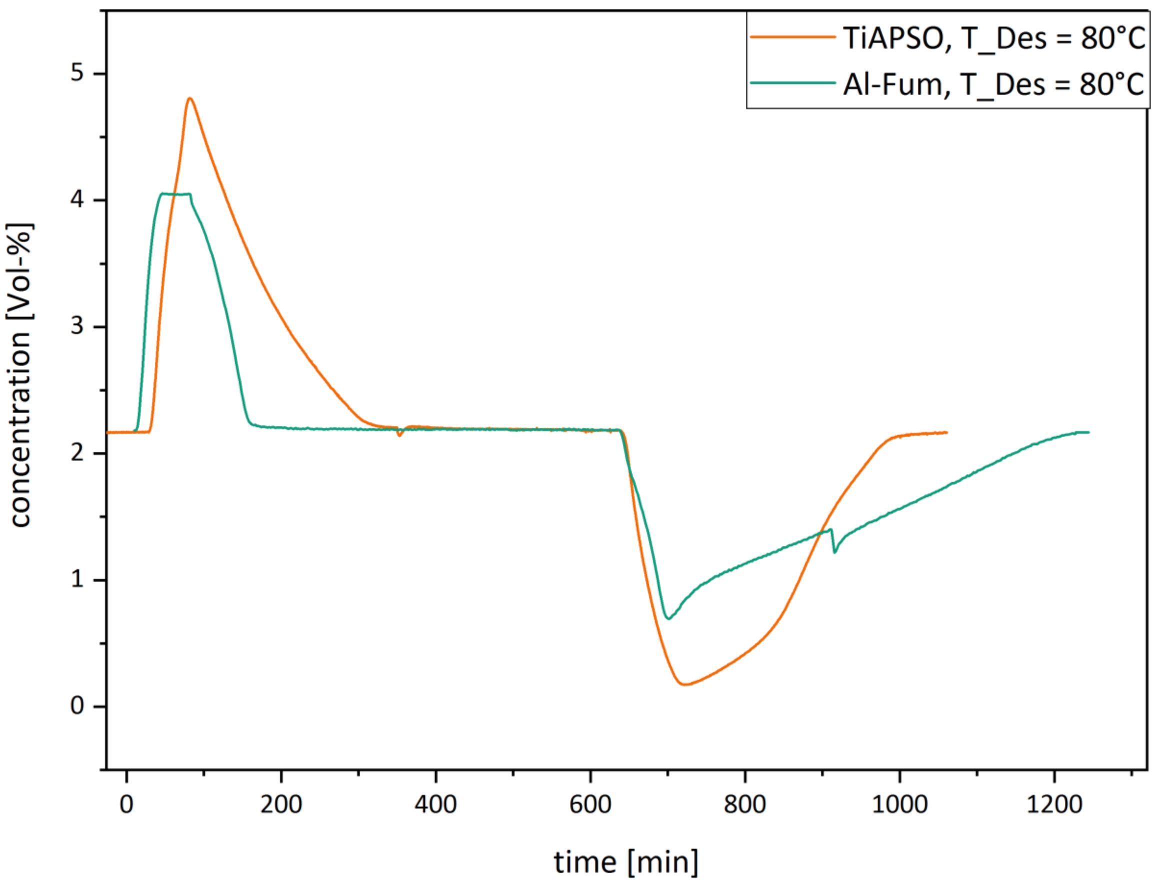
Dynamic Sorption Measurements
Adsorption – Desorption Cycle





- $\dot{V}_{ges}$ 4500 mL min^{-1}
- 50 % rel. humidity

- T_{ads} = 32°C
- T_{des} = 80°C

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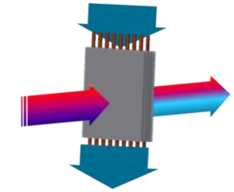
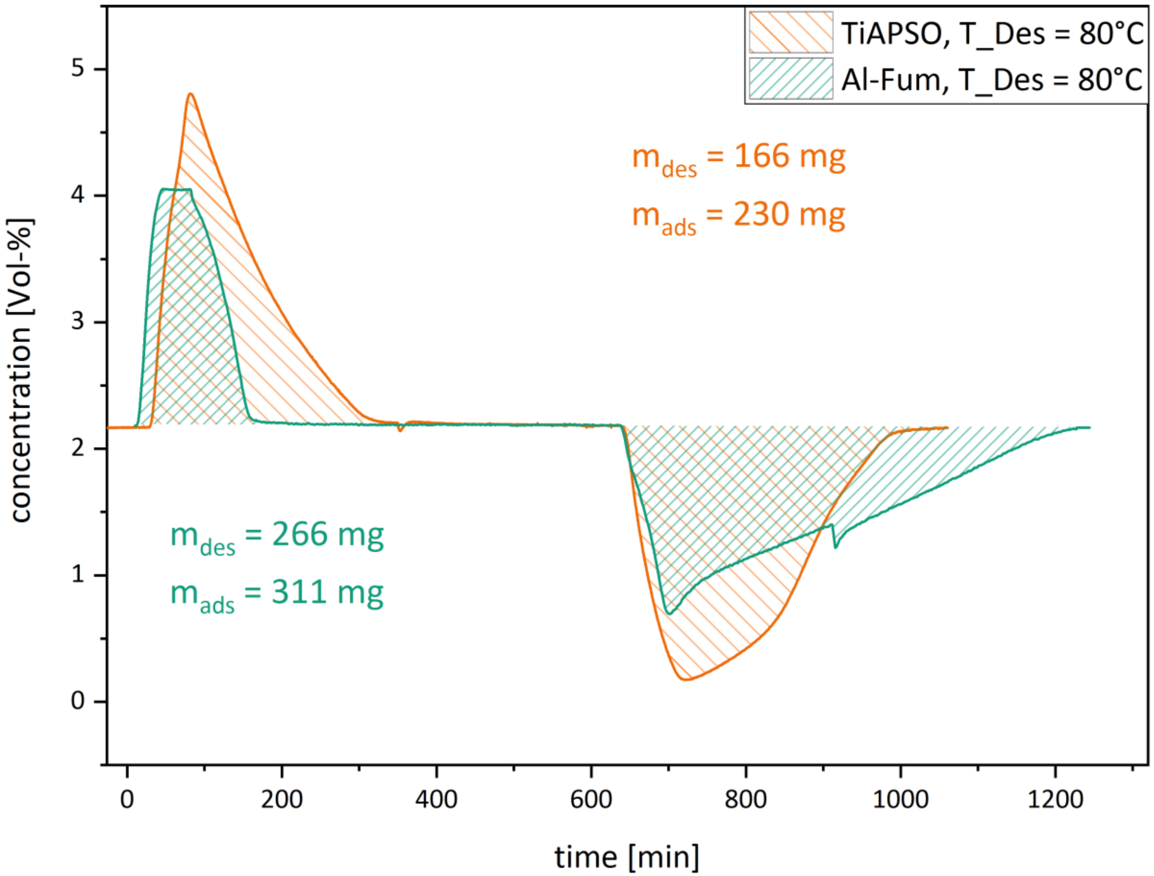
Dynamic Sorption Measurements
Adsorption – Desorption Cycle





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Open applications / gas mixtures
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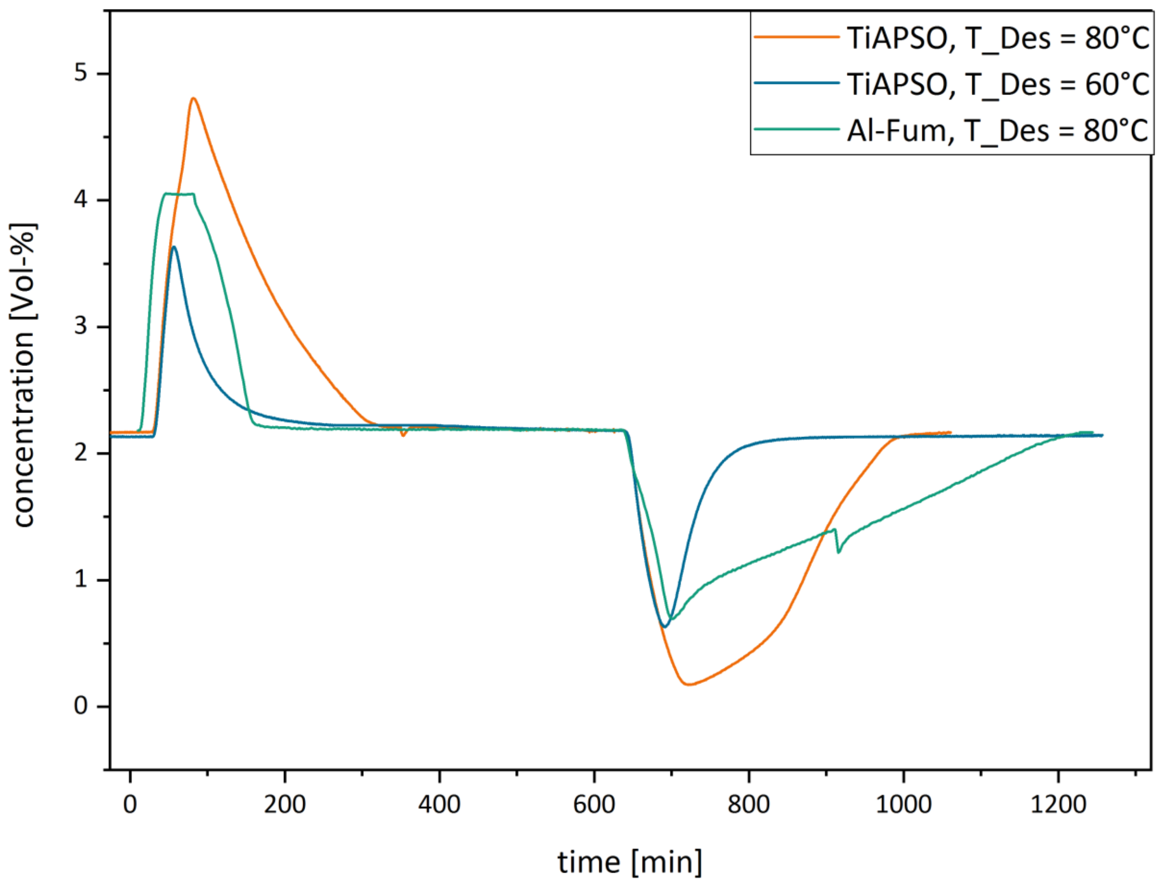

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Conclusion

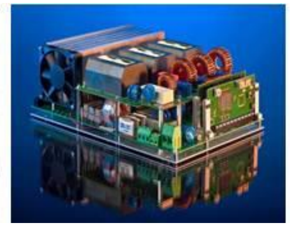
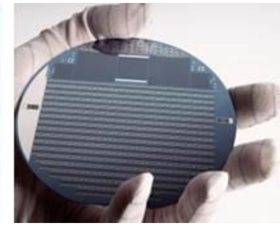
Closed application:

- Non-isothermal effects are severely influencing derived diffusion parameters
- LPJ and LTJ (+ Inert) are serving well for detecting limitations
- Modelling allows extrapolation to different composite/material and application conditions

Open application:

- Breakthrough experiments deliver the right choice of materials for single and multicomponent adsorption

Thank you for your attention!

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