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Non-Isothermal Kinetics of Water Adsorption in Compact Adsorbent Layers on a Metal Support

Modelling in Comsol Multiphysics

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Research on Adsorbent Layers - Motivation

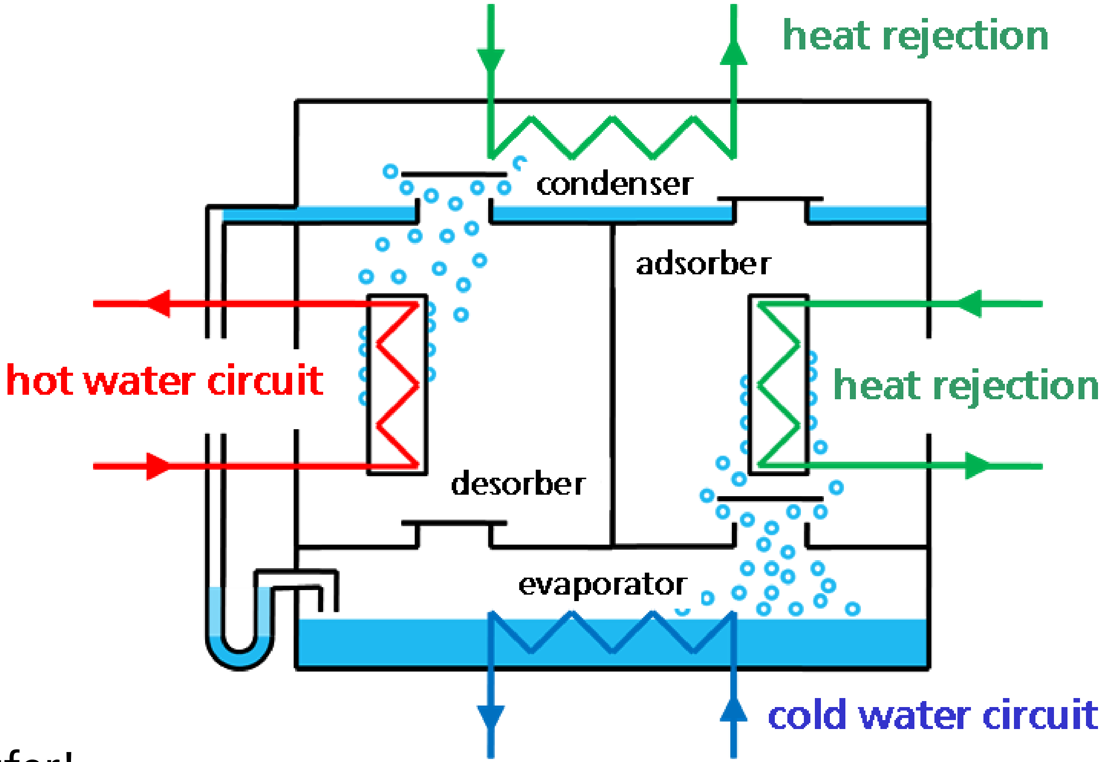
R & D for adsorption cooling machines driven by solar or waste heat

Focus on:

- Adsorbent materials
- More efficient adsorber structures
- Short cycle times, high uptake = high power density

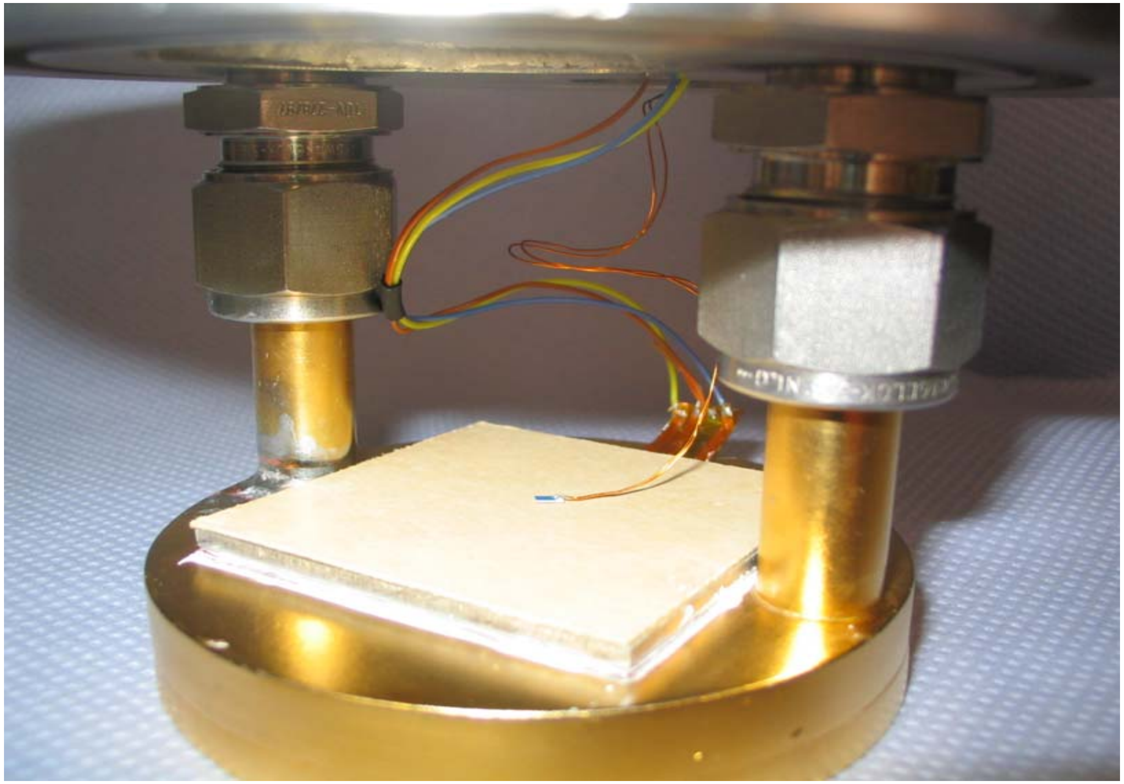
Optimization needs detailed

understanding of heat and mass transfer!



Measurement of adsorption kinetics

- Heat flux to coldplate
- Pressure drop in chamber
- Surface temperature



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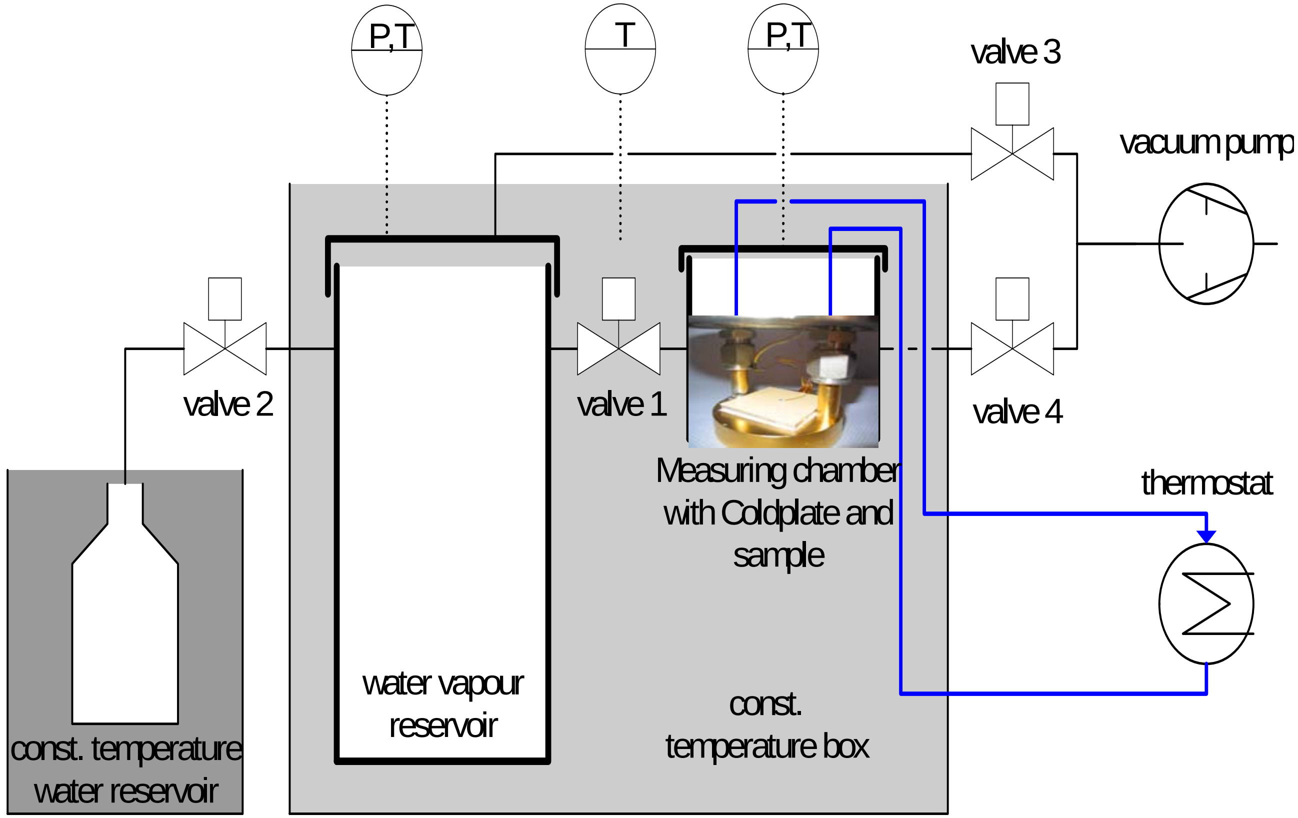
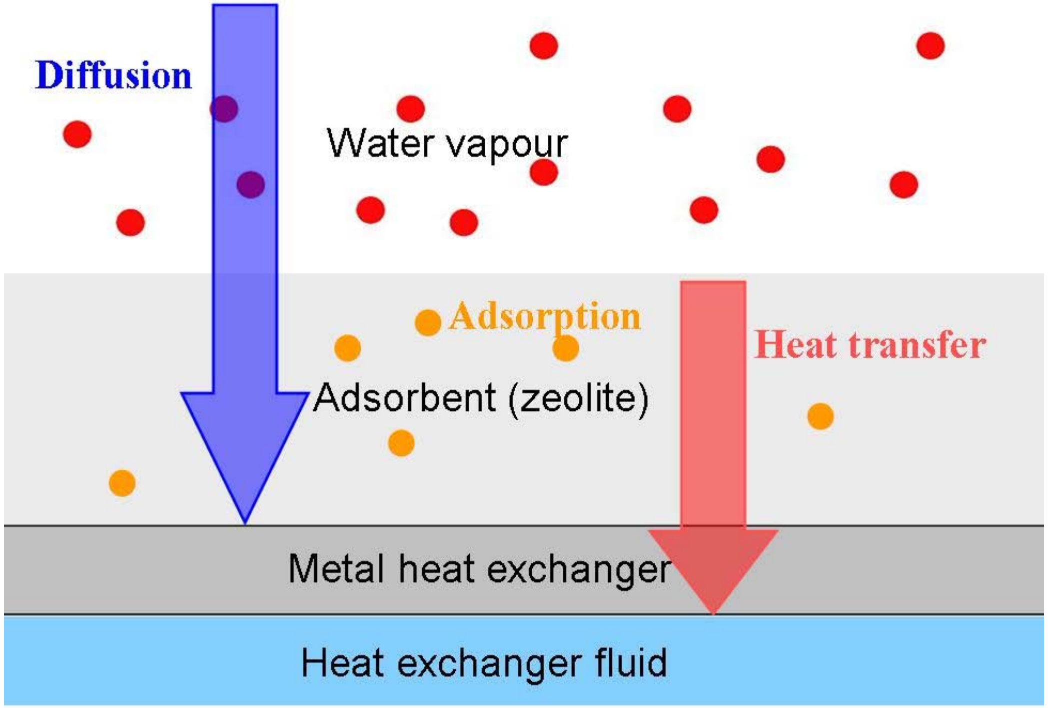


Coupled heat and mass transfer during adsorption



- Water vapour (10-40 mbar)
- Mass transfer by Knudsen diffusion
- Heat transfer by conduction

Model assumptions

- 1-dimensional modelling
- Adsorption equilibrium X(p,T) reached instantaneously
- Water vapour = ideal gas
- Heat transfer by convection in pores ignored
- No heat losses to environment by radiation/convection/conduction

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Coupled set of PDE's

- Mass balance (adsorbent)

$$\frac{\partial c_{Ad}}{\partial t} = \frac{\partial}{\partial z} D \frac{\partial c_{Ad}}{\partial z} - \frac{1}{M} \frac{\rho_{Ad}^{dry}}{\psi} \frac{\partial X}{\partial t}$$

From adsorption equilibrium data

$$\frac{\partial X}{\partial t} = \left(\frac{\partial X}{\partial p}\right)_T \frac{\partial p}{\partial t} + \left(\frac{\partial X}{\partial T_{Ad}}\right)_p \frac{\partial T_{Ad}}{\partial t}$$

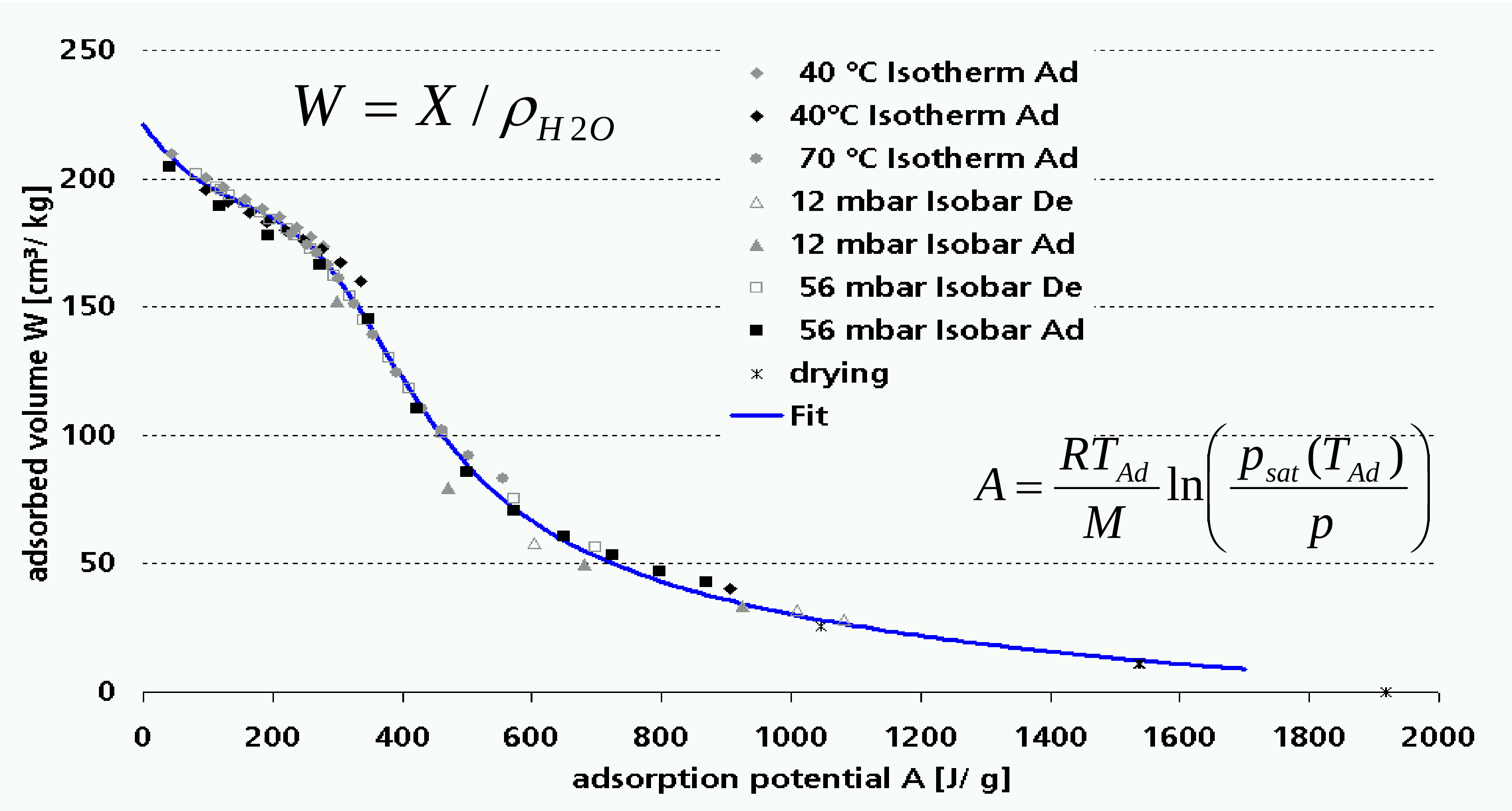
$$p = c_{Ad} R T_{Ad}$$

- Energy balance (adsorbent)

$$T_{Ad,\log} = \ln T_{Ad}$$

$$\delta_{ts} \rho_{Ad,v}^{dry} c_{p,Ad} \frac{\partial T_{Ad,\log}}{\partial t} = \nabla \overline{\lambda}_{Ad,\log} \nabla T_{Ad,\log} + \rho_{Ad}^{dry} h_{ad} \frac{\partial X}{\partial t}$$

Adsorption equilibrium – Dubinin's characteristic curve



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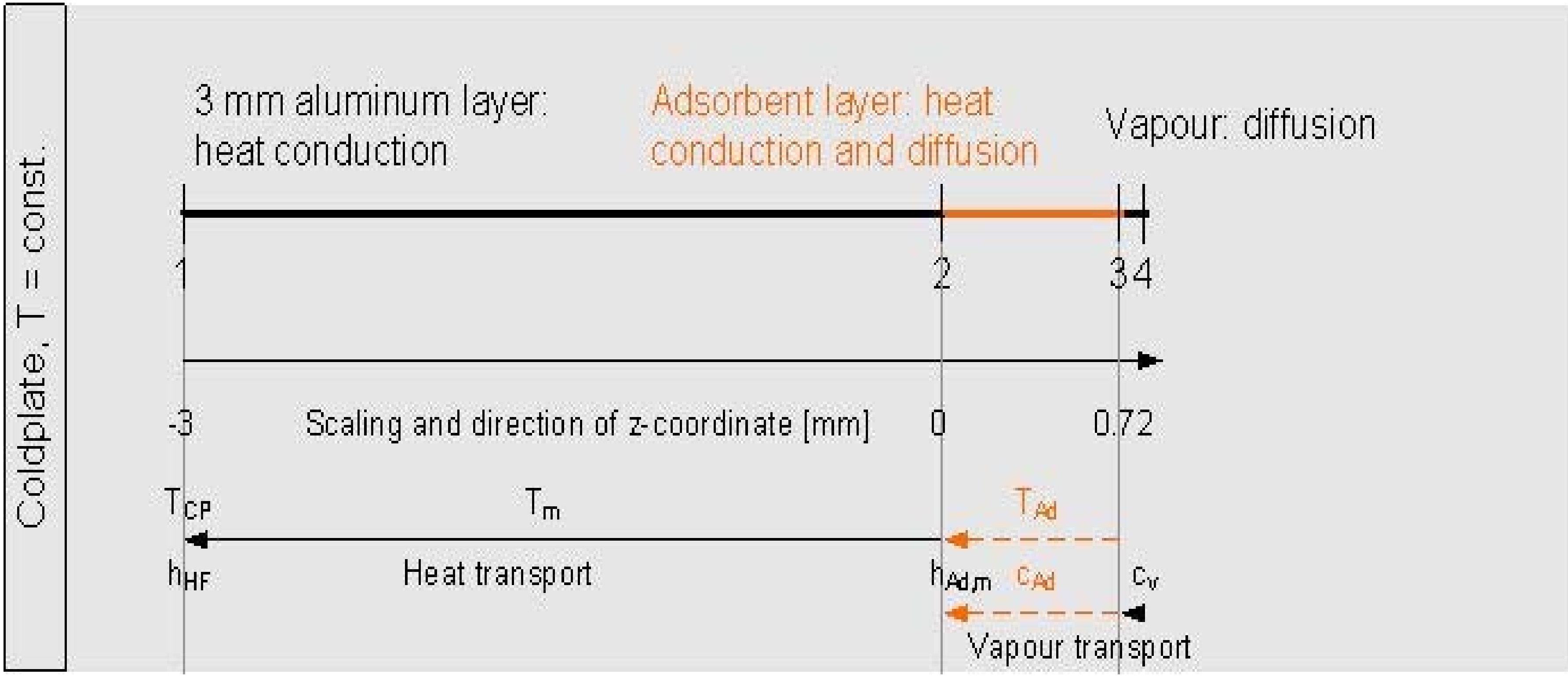
1-D model in COMSOL with boundaries



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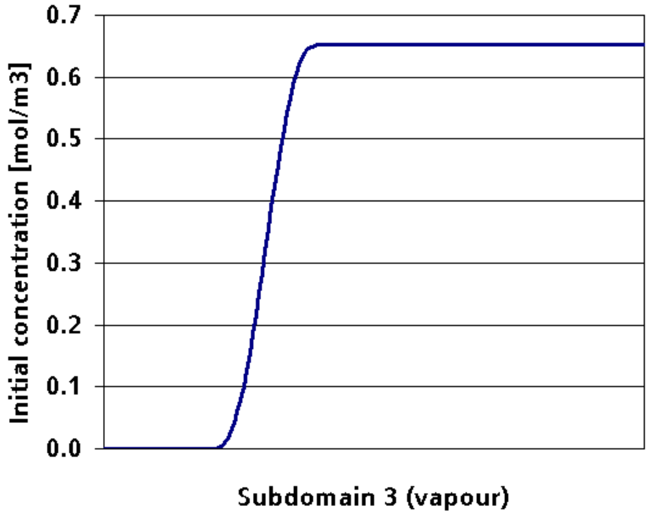
Initial and boundary conditions

- Vapour layer initial concentration (subdomain 3)

$$c_v(0) = c0 - (c0 - c_{Ad}0) * \mathrm{flc2hs}(7.5\mathrm{e}-4 - x, 1\mathrm{e}-5)$$

$$D_v = 0.01 - (0.01 * \mathrm{flc2hs}(3 - t, 3))$$

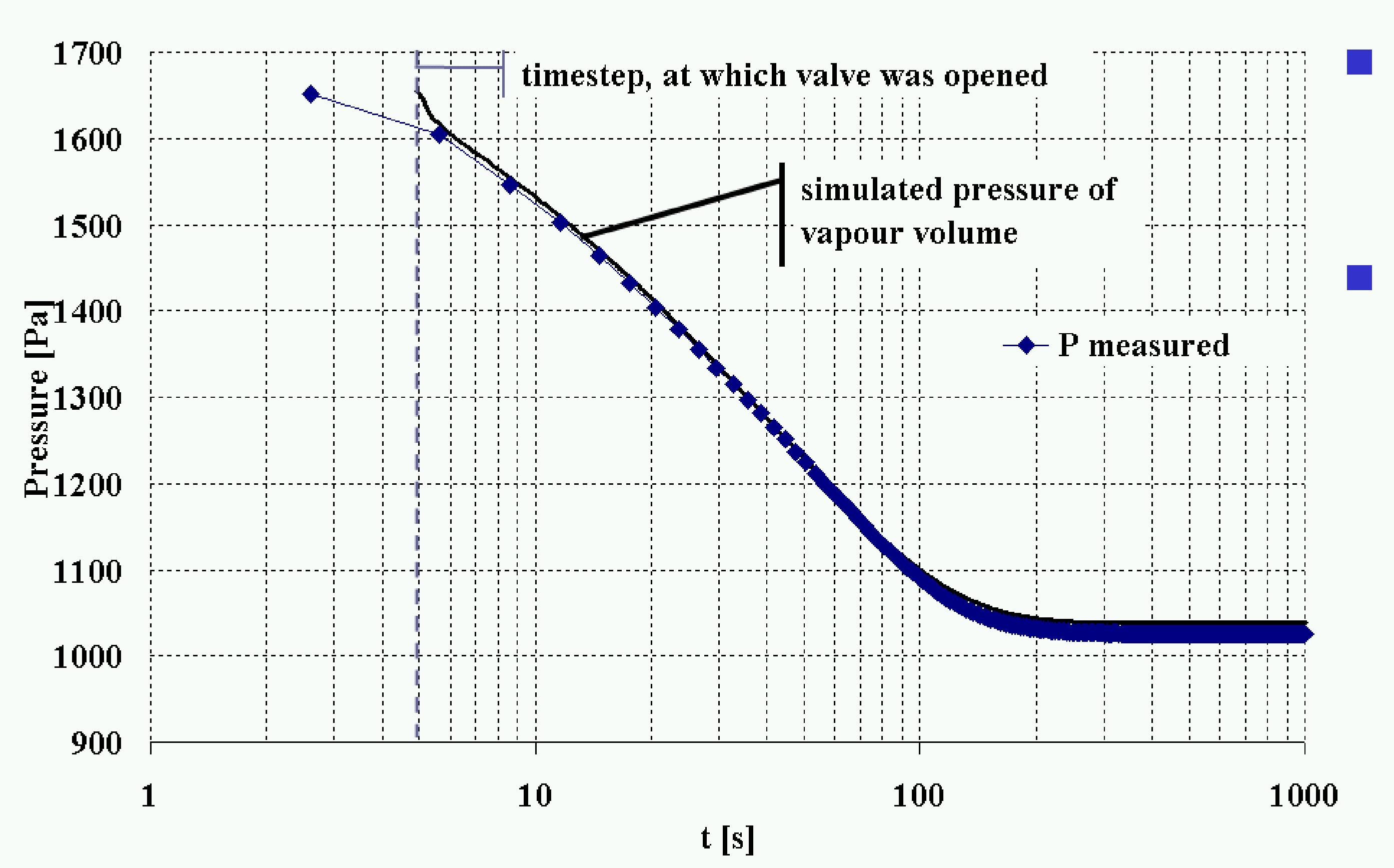


- Vapour layer boundary condition (boundary 4)

$$\mathrm{n}(D_v \nabla c_v) = -\frac{V_{tot}}{\Psi * Area} \frac{\partial c_v}{\partial t}$$

(Flux through surface)

Pressure in vapour volume



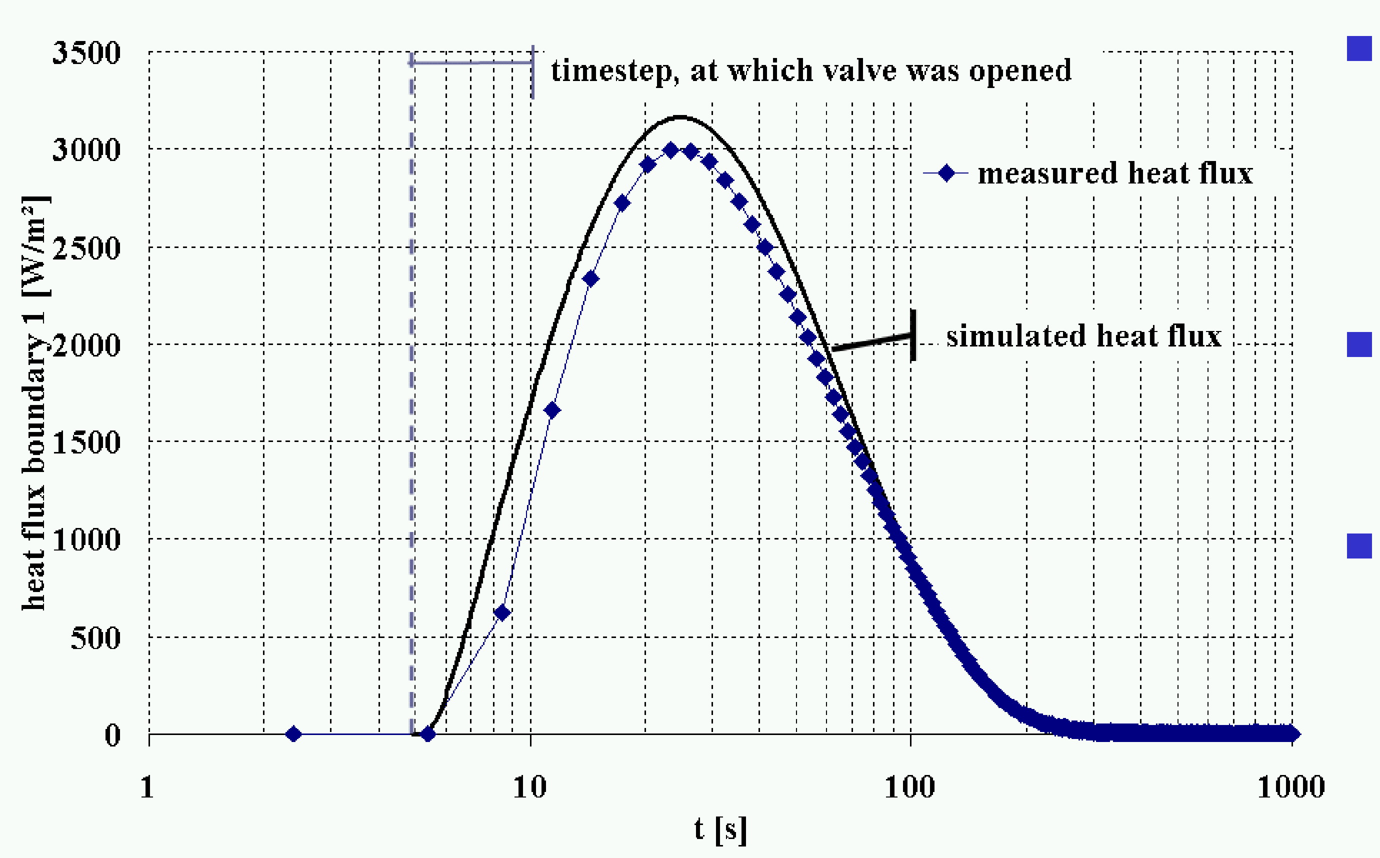
- Constant diffusion coefficient

$$D = 1.1\text{e}-4\,\text{m}^2/\text{s}$$

- Porosity

$$\Psi = 0.42$$

Heat flux to coldplate



- Heat transfer coefficients

$$h_{HF} = 400\,\mathrm{W/m^2K}$$

$$h_{Ad,m} = 500\,\mathrm{W/m^2K}$$

- Thermal conductivity adsorbent

$$\overline{\lambda}_{Ad} = 0.2\,\mathrm{W/mK}$$

- Specific heat capacity adsorbent

$$c_{p,Ad} = (1+3.5*X)\,\mathrm{kJ/kgK}$$

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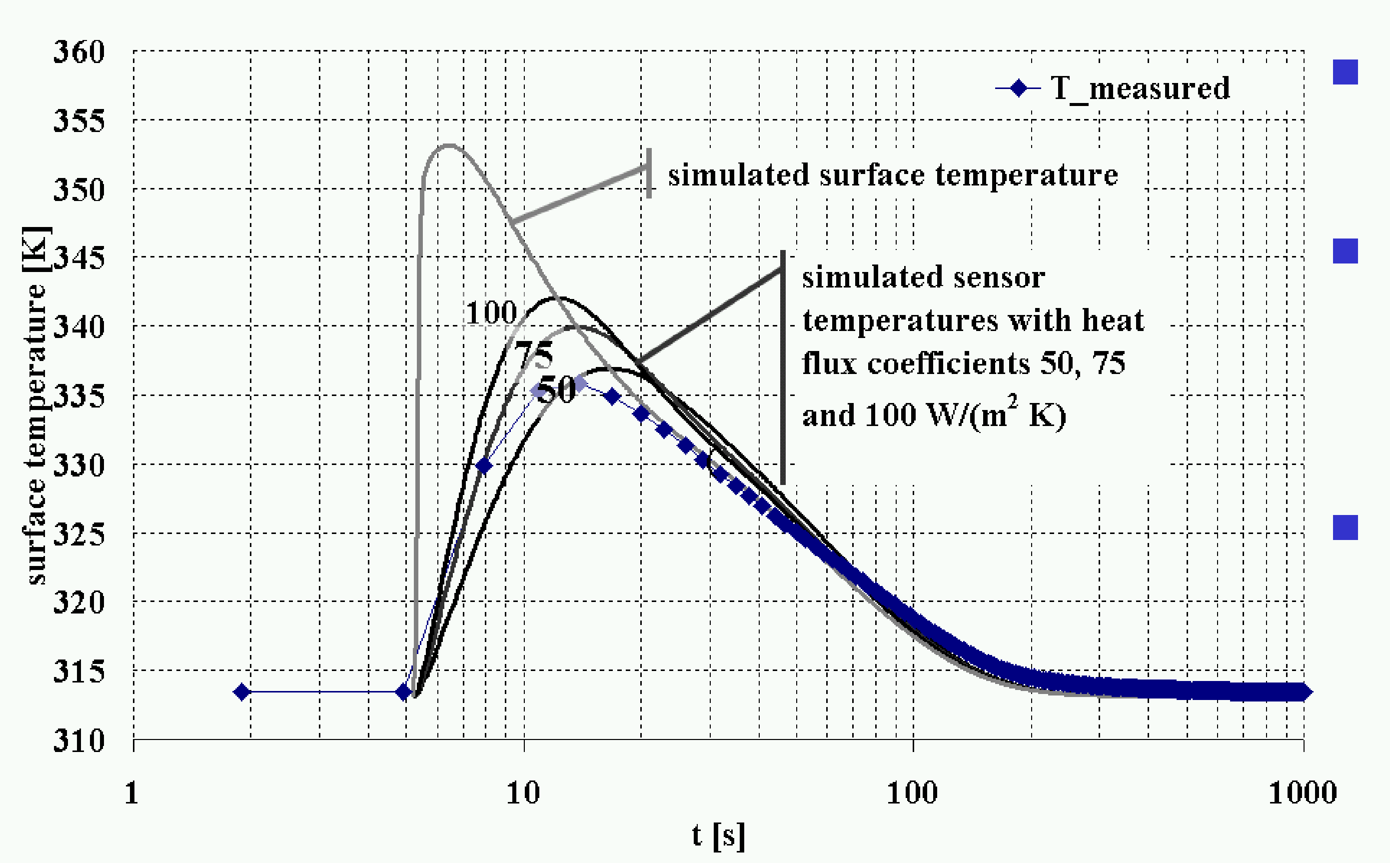
Surface temperature



- Dynamic behaviour of temperature sensor (Ni 100)
- Simulation shows higher maximum temperature peak (353K vs. 336K) within first second!
- Validation necessary by different measurement (e.g. infrared sensor)

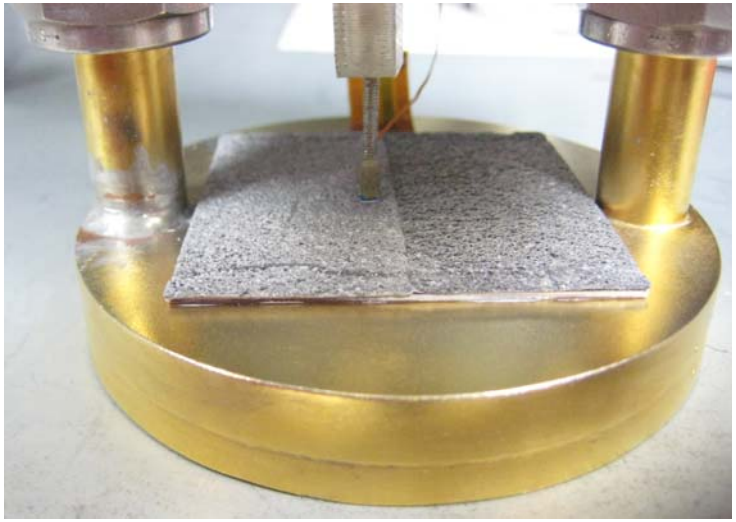
Conclusions

- 1-d model of non-isothermal adsorption kinetics has been set up in COMSOL Multiphysics and validated by experimental data
- Calculation with logarithmic temperature and smoothed initial conditions avoid numerical problems
- Simulation shows higher surface temperature maximum than measurement due to heat flux resistance of temperature sensor

  → different temperature measurement proposed!

- Model can now be used for parameter variation/optimization

Thank you for your attention!



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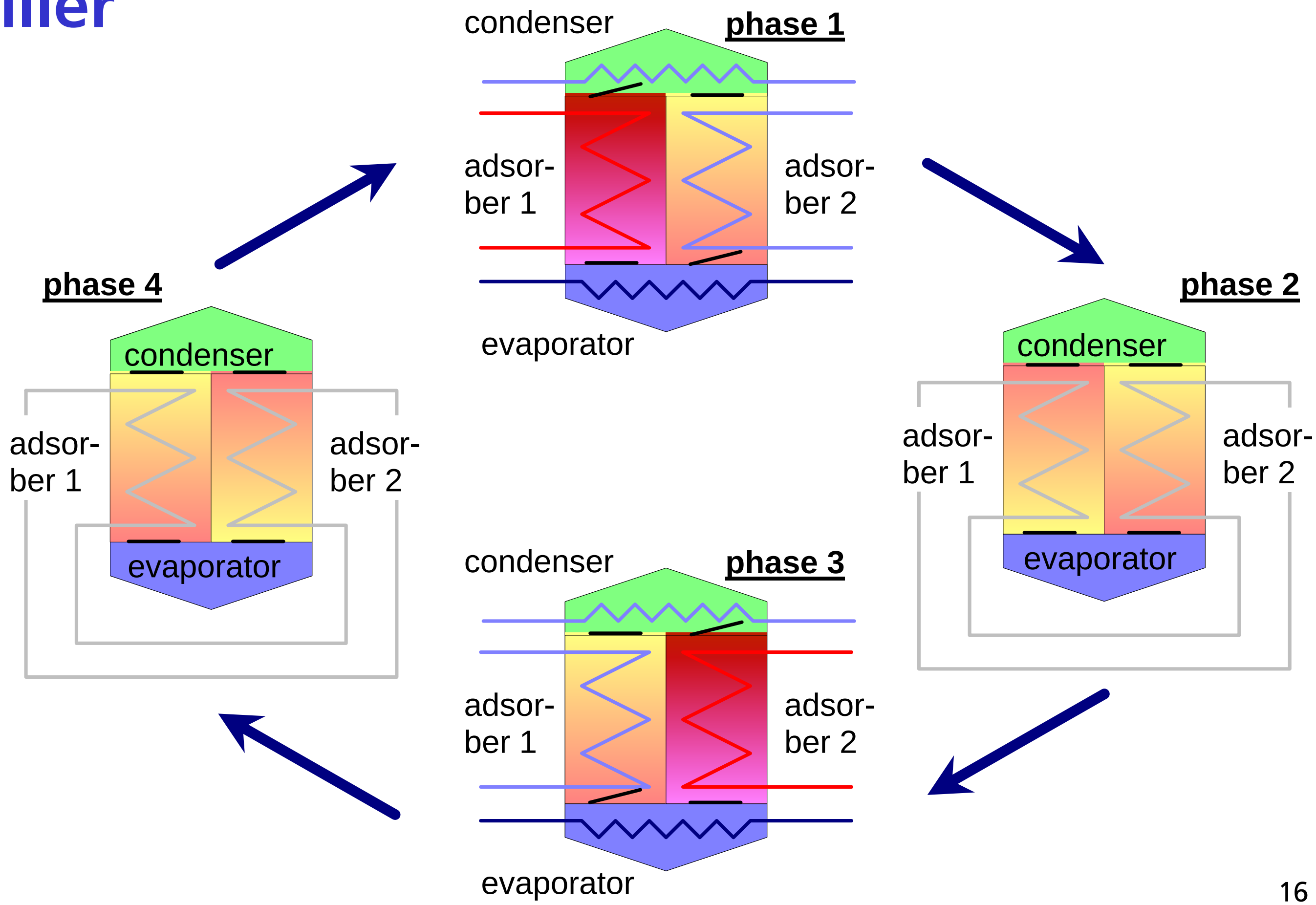
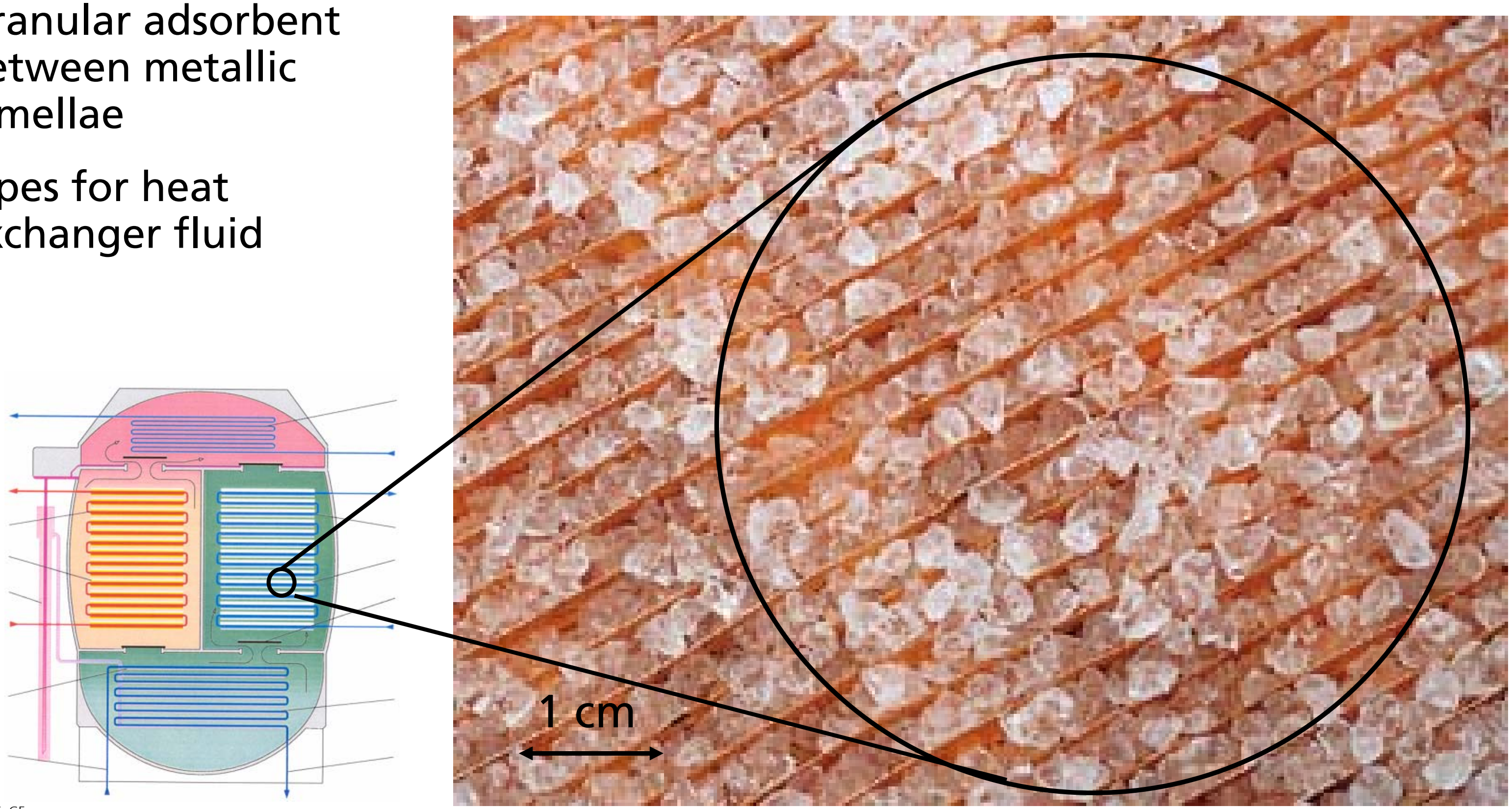
Adsorption chiller



Adsorber: State of the art

- Granular adsorbent between metallic lamellae
- Pipes for heat exchanger fluid



Goal to be reached

Higher volume specific power density of at least 100 W/liter
(COP at least 0,6)

5 W/liter

Goal: 100 W/liter