

Supporting Information

Carbon-Methanol Based Adsorption Heat Pumps: Identifying Accessible Parameter Space Employing Carbide-Derived Carbon as Model Material

Lisa Träger, Jan Gläsel, Marc Scherle, Julian Hartmann, Prof. Dr.-Ing. Ulrich Nieken and Prof. Dr.-Ing. Bastian JM Etzold*

Correspondence: bastian.etzold@tu-darmstadt.de

Technical University of Darmstadt, Department of Chemistry, Ernst-Berl-Institut für Technische und Makromolekulare Chemie, 64287, Darmstadt, Germany.

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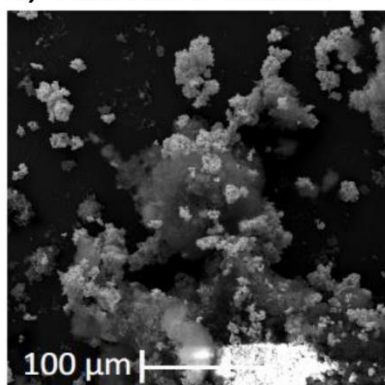
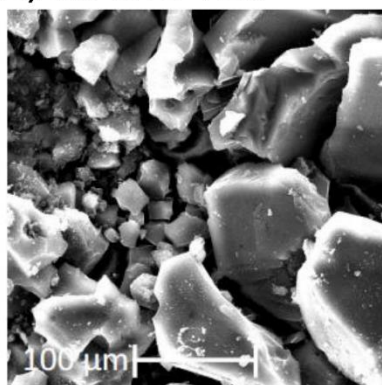
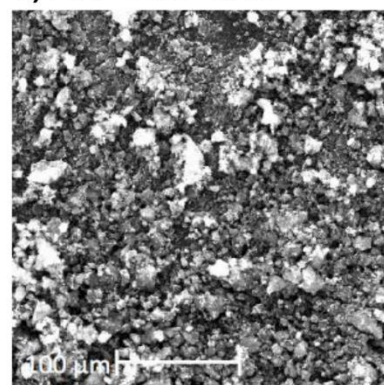
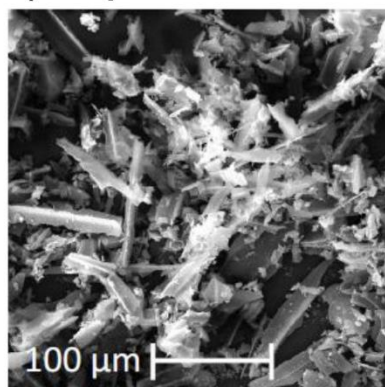
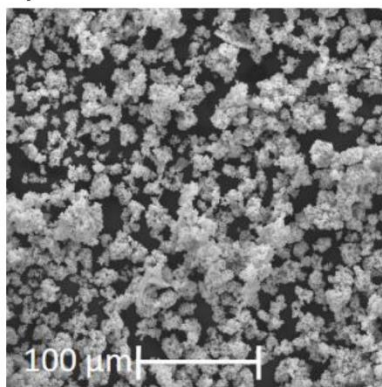
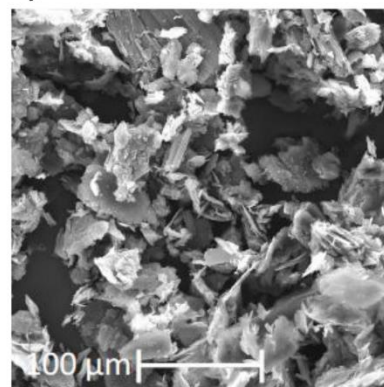
Material Characterization – SEM Imaging**A) Activated Carbon****B) TiC-CDC-1000****C) ZrC-CDC-1000****D) Graphite****E) Boron nitride****F) Silver**

Figure S1. SEM-images of the active materials (A)-(C) and the heat conductive additives (D)-(F) taken at a magnification of 500x.

Adsorption Equilibrium with Static-Volumetric Method – Dubinin-Astakhov Adsorption Isotherm

Experimental setup:

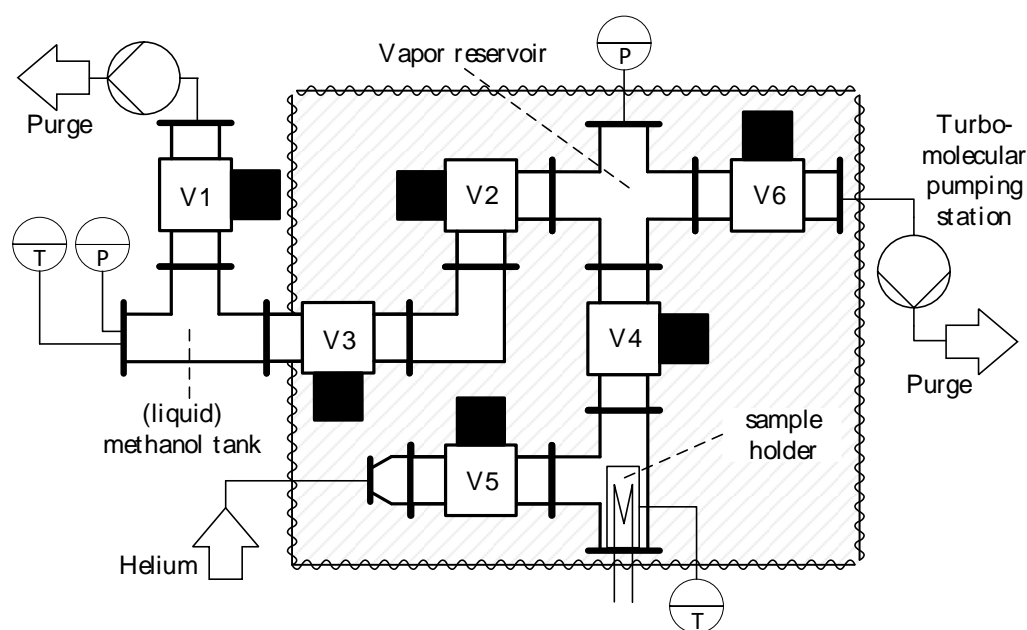


Figure S2. Experimental setup for equilibrium adsorption measurements.

A schematic sketch of the self-developed experimental setup is shown in **Fig. S2**. The setup consists of ultra-high vacuum components in order to minimize gas leakage from the surrounding. All relevant components are embedded in an actively, temperature-controlled (external thermostat), isothermal aluminum bed. The temperature of the sample holder can further be actively controlled with a second, external thermostat. A temperature-controlled pressure transducer serves to detect the MeOH vapor-pressure in the vapor reservoir.

Execution and evaluation of experiments:

After evacuating the setup with a turbo-molecular pumping station ($\approx 10^{-4}$ mbar) and desorbing the sample on the sample holder, vaporous methanol is dosed into the vapor reservoir via V2 and V3 up to a certain vapor-pressure. The MeOH is provided from the methanol tank. By opening of V4, methanol enters the sample chamber and is adsorbed by the sample. After a certain time, the equilibrium is reached, and the amount adsorbed can be calculated from the known chamber volumes and the pressures in the beginning of the experiment and in equilibrium. Using Dubinin-Astakhov's adsorption isotherm, equilibrium experiments over a wide range of temperature and pressure can be described with three fitting parameters W_0, E, n .

$$W = W_0 \cdot \exp\left(-\left(\frac{A}{E}\right)^n\right) \quad (\text{S1})$$

$$A = RT \ln\left(\frac{p^{\text{sat}}}{p^v}\right) \quad (\text{S2})$$

- n : Characterizes the surface heterogeneity
- E : Characteristic energy of one adsorbate
- W_0 : Maximum volume, adsorbate can occupy
- A : Adsorption potential
- $p^{\text{sat}}(T)$: Saturation pressure
- p^v : Equilibrium vapor pressure in the sample chamber

Mass Transfer Measurement with Simplified Wicke-Kallenbach Cell – Dusty-Gas Model

Experimental setup:

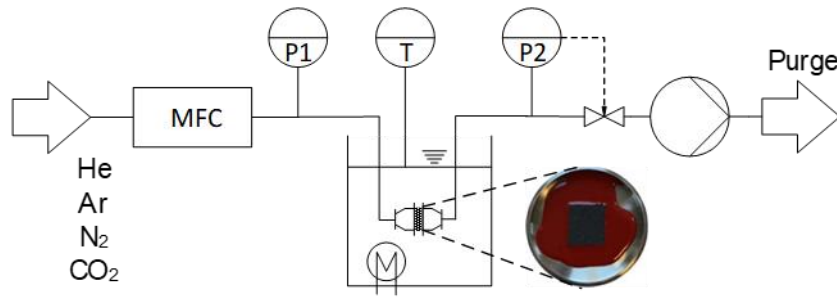


Figure S3. Simplified Wicke-Kallenbach Cell for mass transport measurements.

A simple setup is used to carry out flow experiments. A schematic sketch of the experimental setup can be seen in **Fig. S3**. A defined volume flow of non-adsorbable gases can be provided with a mass flow controller. The supplied gas flows through the sample, which is heated to a defined temperature. The pressure drop across the sample is detected with two absolute pressure transducers. To be able to carry out experiments over a wide flow regime, a vacuum pump has been installed at the end of the experimental setup and a pressure control was installed to regulate the pressure behind the sample (P2).

Execution and evaluation of experiments:

The flow experiments for each sample was carried out with four different, non-adsorbable gases (He, Ar, N_2, CO_2) with a wide variety of molecular masses. For each gas, the experiments were carried out with three temperatures and in each case for six different mean pressures. With the known geometrical parameters of the sample, cross-sectional area (A_p) and sample thickness ($\Delta\xi$), the experiments are evaluated using the Dusty-Gas model (without Stefan-Maxwell diffusion).

$$\frac{RT\Delta\xi\dot{N}_j}{\Delta p A_p} = \frac{\epsilon_p D_j^{Kn}(T)}{D_j^{Kn,eff}(T)} + \frac{\epsilon_p B_0}{B_0^{eff}/\eta(T)} \frac{p_1 + p_2}{2} \quad (S3)$$

$$\frac{R\sqrt{T}\Delta\xi\dot{N}_j}{\Delta p A_p} = \underbrace{D_j^{Kn,eff}(T)/\sqrt{T}}_{D_j^{Kn,const}} + \frac{B_0^{eff}}{\eta(T)\sqrt{T}} \frac{p_1 + p_2}{2} \quad (S4)$$

$$\text{with:} \quad \dot{n}_j = \dot{N}_j / A_p \quad (S5)$$

$$\text{and} \quad D_j^{Kn}(T) = \frac{4}{3} r_p \sqrt{\frac{2RT}{\pi MW_j}} \quad (S6)$$

This linear correlation allows the identification of the effective permeability (B_0^{eff}) from the slope (multiplied with the kinetic viscosity) and the constant part of the Knudsen diffusion coefficient ($D_j^{Kn,const}$) from the intersection with the ordinate. The values determined for the experiments with the three temperatures were averaged. An exemplary evaluation for a plate with TiC-CDC-1000 (75-150 μm ; 5 wt.-% CMC) can be seen in **Fig. S4**.

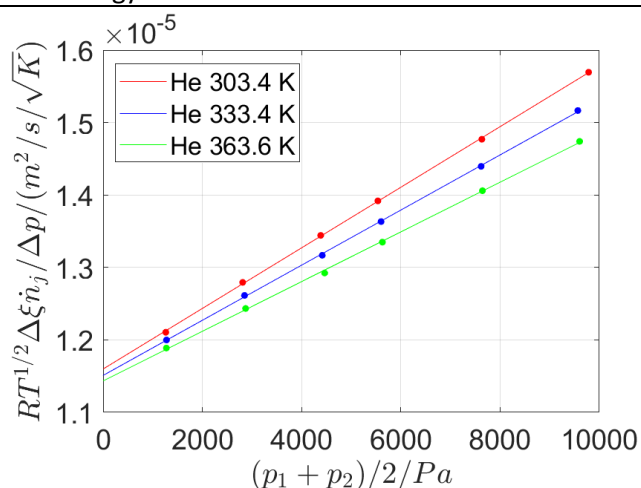


Figure S4. Plate with TiC-CDC-1000 (75-150 μm ; 5 wt.-% CMC): Evaluation according to the Dusty-Gas model.

Since the permeability is solely structure-dependent, the values obtained for the four gases should be the same which was the case for most of the samples. Here, we averaged the values obtained for the four gases to a final, effective permeability. These values are listed in **Tab. 2**.

Besides a structural dependence, the constant part of the Knudsen diffusion coefficient is dependent on the reciprocal value of the square root of the molecular mass of the gas. This dependency is widely known as Graham's law and is visualized in **Fig. S5**. The value for Methanol is interpolated from this linear dependency and the values for different samples are listed in **Tab. 2**.

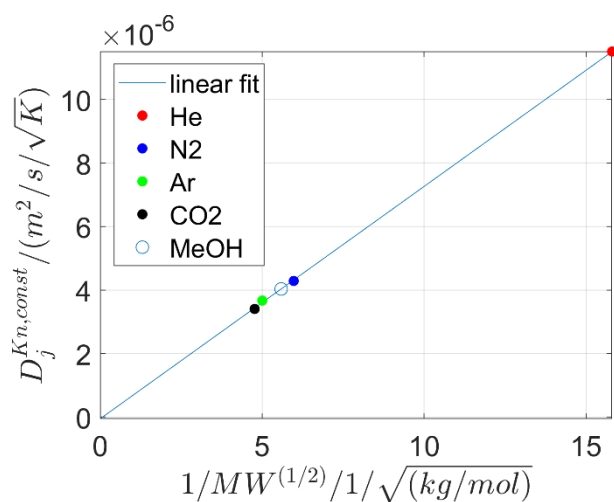


Figure S5. Plate with TiC-CDC-1000 (75-150 μm ; 5 wt.-% CMC): Determination of the constant part of the Knudsen diffusion coefficient for MeOH.