

Adsorption-Liquid-Isotherms on Activated Carbon Fiber Cloth

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1 Abstract

An innovative apparatus and a new method of adsorption equilibria measurements are described. On the basis of the results obtained, the new adsorbate-liquid-isotherm (ALI) model determines the relevant model parameters for further evaluations. The results obtained for a total of eight adsorptives, toluene, n-pentane, n-octane, propanole-2, acetone, and isobutyl glycol ether acetate on micro-porous activated carbon fibre cloth (ACC) and for ethyl acetate and water on micro-porous activated carbon fibre cloth as well as on micro- and meso-porous activated carbon granulate (GAC) will be presented. The new measurement apparatus will be described in conjunction with the results of measurements carried out at temperatures of 45°C to 180°C with $\sim 5\text{mg/m}^3$ to $\sim 200,000\text{mg/m}^3$ gas loading. The measured values can be fitted to one single thermodynamically consistent equation, with an accuracy of 92% to 98%. This adsorbate-liquid-isotherm (ALI) equation also satisfies the boundary conditions for both the Langmuir and the Dubinin-Asthakov equations, as well as those of Henry's law.

2 Introduction

Processes based on adsorption from the gas phase are used e.g. in industrial plants for solvent recovery, for separation or enrichment of volatile organic components and industrial gases, and as filters for the ventilation of buildings and production facilities. Adsorbents are used in gas-chromatographic analysis as well as in private areas, e.g. in automotive interior air intake filters, in self-protection masks and in kitchen exhaust air filters. The solvent concentration in the gas phase for these processes covers a range of some $\mu\text{g/m}^3$ for air intake filters to several kg/m^3 in pressure swing adsorption systems.

Solvent recovery by adsorption, e.g. on activated carbon, is one of the oldest and best-proven processes for exhaust air decontamination. After many decades of practical application, it is astonishing to see that many manufacturers and users of such systems and processes, including the adsorbent manufacturers, still lack considerable knowledge on the basics of the adsorption process. When more than pure empirical knowledge is required, this lack of knowledge includes both the process-technical design for optimal operation and the evaluation of limiting or restrictive secondary parameters.

One of the main reasons is certainly that this subject is relatively complicated and complex. Furthermore, in the past energy efficiency had no great importance and experimental investigations into the subject under reality-oriented conditions were and still are very time-consuming. Even the most basic information needed for understanding and optimising operational processes, namely reliable measurement of adsorption isotherms for the entire, relevant concentration and temperature ranges, is only very rudimentary.

Our investigations and results are intended as a contribution towards the remedy of this deficit. If adsorption technology advances at a real engineering level, it will be applied in practice more often than before and above all, be more efficiently and reliably. To mention one example: the energy saving potential for the decontamination of slightly contaminated exhaust air is far from being realised.

By the results of our isotherm field measurements and the parameters derived from these with the ALI equations, we can e.g. calculate break-through curves, desorption gas concentrations, activated carbon loading profiles and temperatures as a function of place and time. This of course requires suitable process models, validated by measurements, and mathematical algorithms for all material and heat-exchange processes on and in the adsorbent itself, as well for the flow and heat-exchange processes in the adsorption system. With relatively little effort, this would enable the design and optimisation of adsorption processes e.g. in respect of degrees of separation, enrichment factors for desorption and energy consumption.

The following figures illustrate the results of such a process simulation. The example is the decontamination of air from a production facility at an aluminium foundry [1] by an electrically regenerated adsorber with 15 layers of activated carbon fibre cloth (ACC). Because of the competing place and time dependant adsorption and desorption of low boiling point (Dimethyl amine), moderate boiling point (Heptane) and high boiling point (Methyl ethyl benzene) solvents and the strongly fluctuating raw gas concentrations, these relationships were in fact rather complicated. In spite of this, the actual behaviour of the concentrations, temperatures and energy fluxes could be very well described with the models developed. These results will be reported in a

separate article, elsewhere.

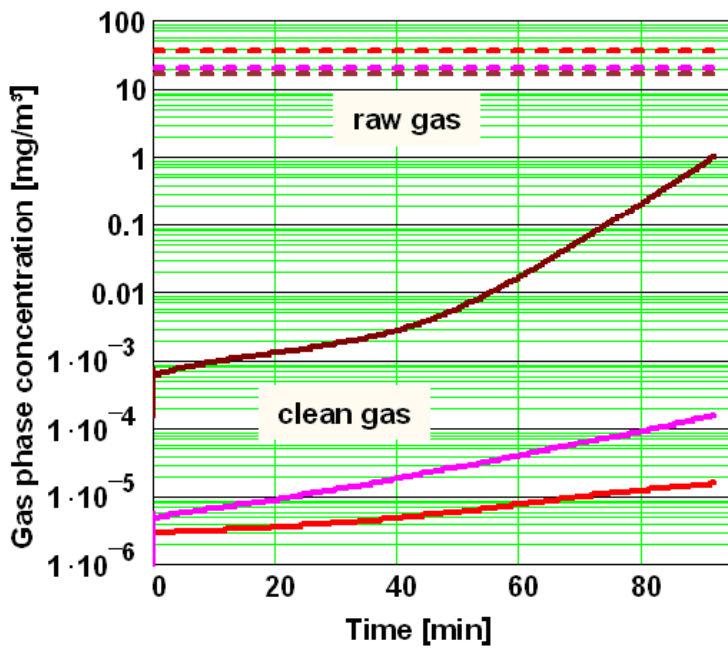


Figure 2.1: Raw gas and clean gas concentrations during the adsorption phase as a function of the adsorption time, red: Methyl ethyl benzene, violet: Heptane, brown: Dimethyl ethyl amine

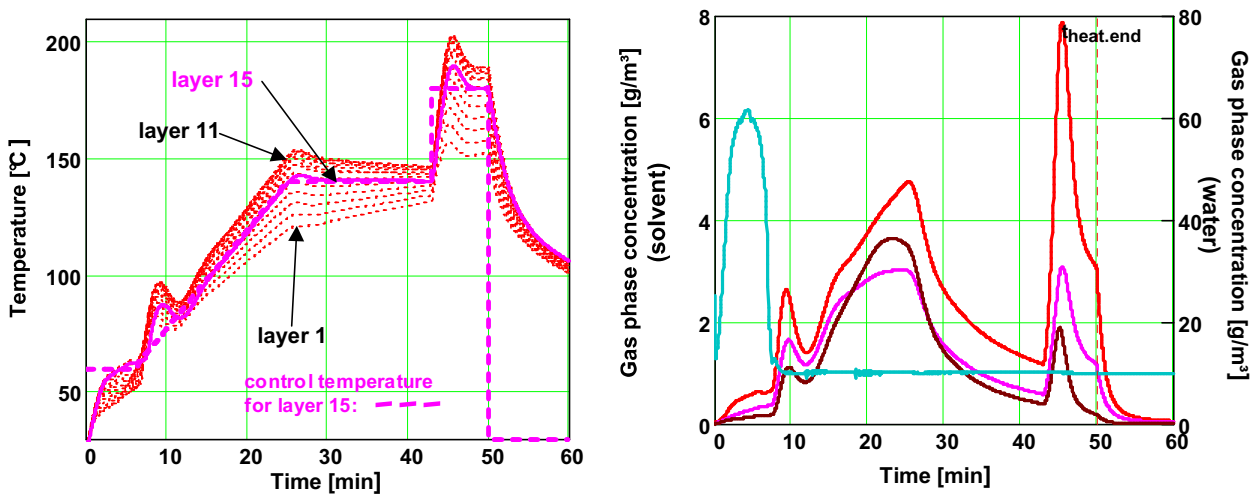


Figure 2.2: **left** – calculated temperature profiles over the 15 activated carbon fibre cloth-layers during the regeneration phase, dotted line - control temperature for the 15th and last cloth-layer exposed to flow, **right** - gas phase concentrations during the regeneration phase, red: Methyl ethyl benzene, violet: Heptane, brown: Dimethyl ethyl amine, blue: water

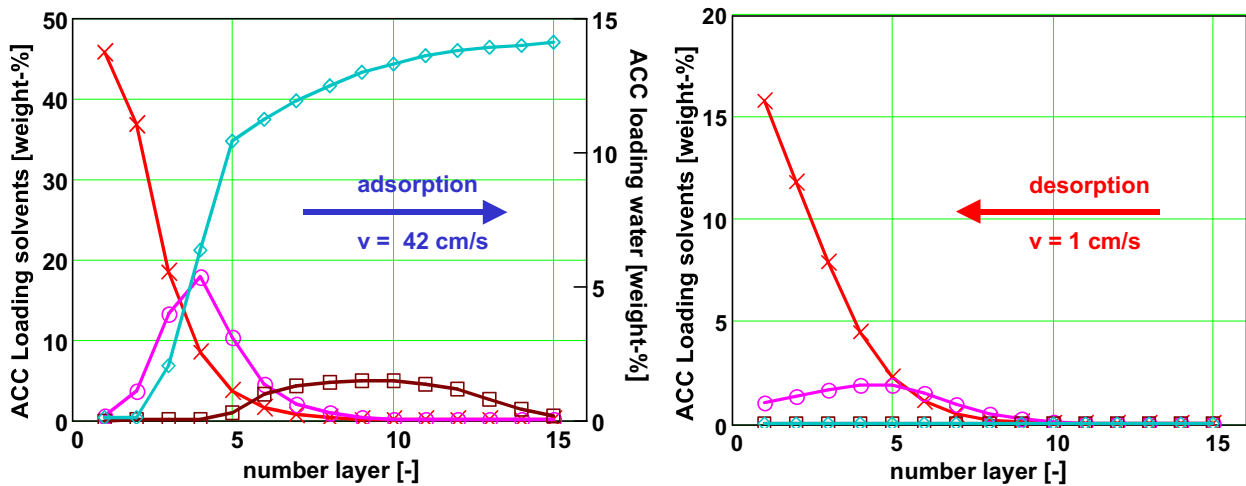


Figure 2.3: Loading profile of the activated carbon fibre cloth (ACC) at the end of the adsorption phase (**left**) and at the end of the regeneration phase (**right**), red: Methyl ethyl benzene, violet: Heptane, brown: Dimethyl ethyl amine, blue: water

3 Equilibrium-Adsorption-Apparatus - Method of Measurement and Results

The equilibrium adsorption apparatus (EAA) is designed to measure the adsorption-isotherms for solvents on adsorbents, here for example of activated carbon fibre cloth. The method allows fast and reliable measurement, see the comparison with previously used methods of measurement in Figure 3.1 and in [2]. With the equilibrium adsorption apparatus, isotherm fields can be measured for all technically relevant solvents with boiling points less than 250°C in a fraction of the time required by conventional methods. The measurement duration for a solvent takes around six hours per isotherm. In all cases, the relative error of the isotherms measured compared to the isotherms determined by extrapolation using the ALI model was less than 10% (the maximum error occurred with water) over the entire range of the pore-filling-degree, i.e. the loading, and the temperature. For the 7 organic solvents tested, the mean relative error was 3.5%. This is completely sufficient for technical purposes in connection with system design and process simulation.

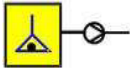

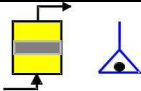
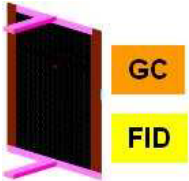
Method	Visualisation	Range of measurement	Time measured
steady-state adsorption balance		$C > 300\text{mg/m}^3$ $T < 65^\circ\text{C}$	one week
flow-through adsorption balance		$C > 1\text{mg/m}^3$ $T < 65^\circ\text{C}$	several weeks
forced-flow apparatus and balance		$C > 1\text{mg/m}^3$ $T < 200^\circ\text{C}$	several weeks
equilibrium adsorption apparatus		$C > 1\text{mg/m}^3$ $C < 300000\text{mg/m}^3$ $T > 45^\circ\text{C}$ $T < 250^\circ\text{C}$	six hours

Figure 3.1: Comparison of methods for the measurement of adsorption isotherms

3.1 Description of the Equilibrium Adsorption Apparatus

In the equilibrium adsorption apparatus, a regulated carrier gas stream is circulated via a closed primary gas loop into the equilibrium adsorption chamber, the adsorber, see figure 3.2. By means of injection, the adsorptive, in general a solvent, is added in an exactly proportioned amount to the carrier gas stream. The gas loop is equipped with an injector, a static mixer, different measuring facilities, and the electrically directly heated adsorber. The direct heating accomplished by means of the ohmic resistance of the activated carbon fibre cloth results in the fact that the solvent is adsorbed at a well defined, exactly controlled adsorbent test temperature.

The entire gas loop is enclosed in a heated, thermally isolated housing. Figure 3.2 shows the schematic flow diagram of the equilibrium adsorption apparatus and Figure 3.3 is a front view. The adsorbent, here the activated carbon fibre cloth, is fixed in an electrically non-conductive frame, stable up to 250°C , and then mounted in the equilibrium adsorption chamber, the adsorber, see Figure 3.4.

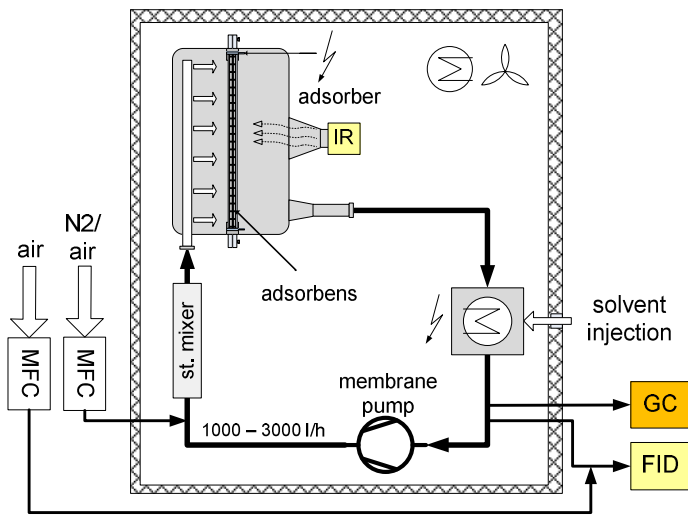


Figure 3.2: Basic flow diagram of the equilibrium adsorption apparatus



Figure 3.3: Front view of the equilibrium adsorption apparatus with insulation shell removed, the yellow pyrometer and its control unit

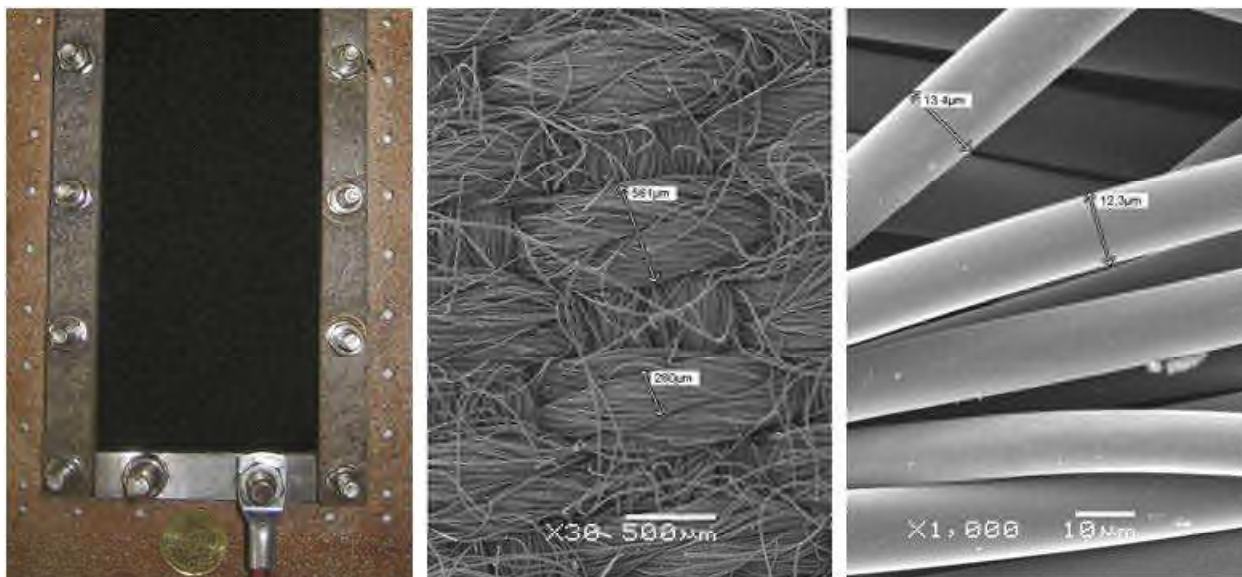


Figure 3.4: Isolated frame, containing the activated carbon fibre cloth with current supply, cloth enlarged 30 times, activated carbon fibres enlarged 1000 times

3.2 Method of Measurement

The carrier gas filled loop as well as the prepared and conditioned adsorbent are brought to the required operating temperature without the introduction of any adsorptive. A special feature is that direct electric heating maintains the activated charcoal fibre cloth at the required measurement temperature within $\pm 0.5^{\circ}\text{C}$. The subsequently injected solvent is transported by the membrane pump through the system and through the adsorbent. The adsorbent becomes loaded with adsorptive. Adsorption takes place until the partial pressures of the adsorptive adsorbed and the free adsorptive in the carrier gas are in equilibrium. The time for this is usually in between 2 to 10 minutes. A defined number of samples is removed from the loop after 3-15 minutes, within a well-defined measurement time of 1-2 minutes. The solvent concentrations in the gas phase are measured with a flame ionisation detector (FID) or a process gas chromatograph (PGC), while maintaining constant system pressure. In order to measure the next higher loading on the isotherm, the next quantity of solvent has to be injected. As an example, Figure 3.5 shows a measurement curve, for an experiment where toluene was injected.

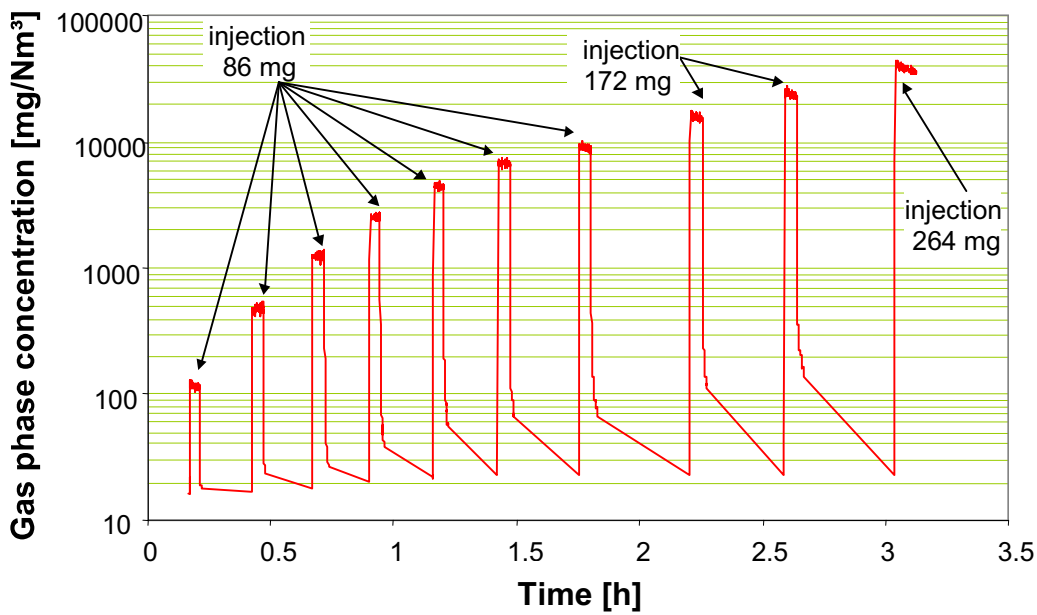


Figure 3.5: Examples of measurement curves for toluene and activated carbon fibre cloth

Each measurement procedure provides its own small series of measured values, characterised by a drop in gas concentration. A few seconds elapse between the start time and the first measuring signal for the concentration measurement. Therefore the extrapolation to the start time of the measurement yields the gas phase concentration used for the calculation of a point on the adsorption isotherm. On the basis of a mass balance, the loading X_{as} of the adsorbent can be calculated e.g. in $[g_a/100g_s]$, see [SiKi1 08] for more details.

For each new temperature a new fabric was used, taken from the same production batch. In preliminary investigations, loading tests with toluene at three gas phase concentrations and mass density determination of the cloth showed that the mean variation range for the maximum loading was $\sim 3.5\%$ and the maximum variation range $\sim 5\%$ over the entire production batch.

3.3 Results of the Adsorption Isotherm Measurements

Table 3.1 summarises a few physical properties of the eight solvents measured on Chemviron FM5/250 activated carbon fibre cloth with the equilibrium adsorption apparatus. With the chosen selection of the solvents measured, a relatively broad range of commonly used industrial solvents is covered.

Solvent	Boiling point [°C]	Solubility in water (hydrophilicity)	Polarity
Toluene	110.7	very low	low
n-Pentane	36.1	very low	low
n-Octane	125.7	very low	low
Propanol-2	82.3	completely miscible	high
Acetone	56.3	completely miscible	high
i-Butyl glycol ether acetate	189.2	low	high
Ethyl acetate	77.2	moderate	moderate
Water	100.0	---	high

Table 3.1: Physical properties of the solvents investigated

3.3.1 Measured Results for Toluene, n-Pentane, n-Octane, Propanol-2, Acetone and i-Butyl glycol ether acetate

As Figure 3.6 below illustrates, for six of the solvents the measurements carried out with the equilibrium adsorption apparatus yield consistent isotherms with only very limited scatter. This is true for the entire, very broad range of measurements from 60°C to 180°C from ~5mg/m³ to ~200,000mg/m³ and for the corresponding pore filling degree Ξ from 1% to 80%. The isotherm for toluene at 35°C was measured by using the conventional forced-flow method for the means of comparison. It can be seen that this isotherm fits smoothly into the isotherm range measured with the equilibrium adsorption apparatus at higher temperatures. Moreover, we can recognise that the measured values can be very well described with the thermodynamically consistent adsorbate-liquid-isotherm (ALI) model for activated carbon fibre cloth over a very broad range of temperatures and over the entire range of pore filling degrees of the adsorbent. The mean relative deviations fall within the fluctuations which one can expect alone from the scatter in quality of the activated carbon fibre cloth. The measurement error increases for concentrations below 5mg/m³ and above 50,000mg/m³. At lower concentrations residual concentrations in the measuring apparatus have greater influence. At very high concentrations, the difference between the amount of injected solvent and the operational solvent level in the gas phase of the apparatus yields to a very small value.

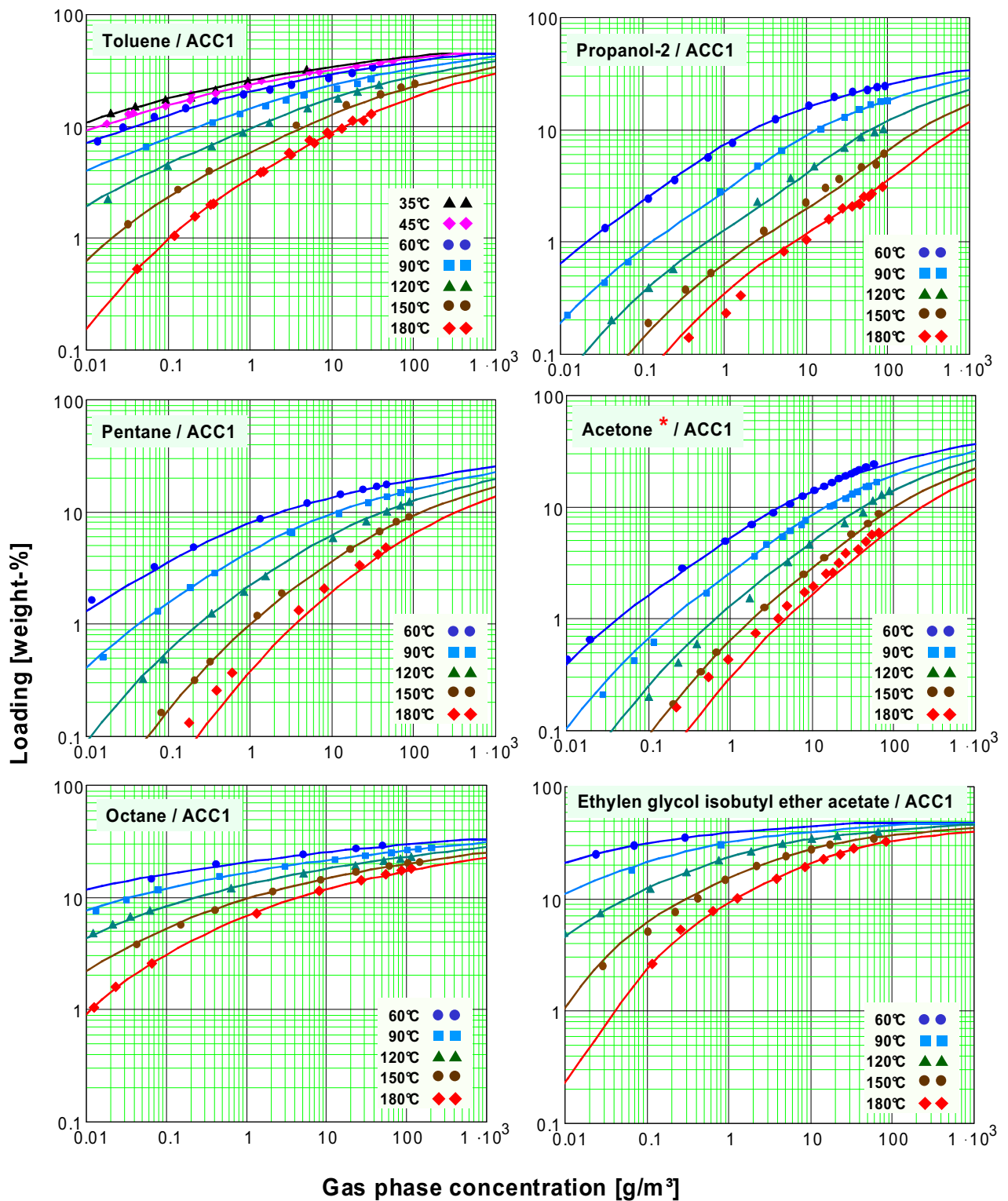


Figure 3.6: Adsorption isotherms of toluene, n-pentane, n-octane, propanole-2, acetone* and i-butyl glycol ether acetate on activated carbon cloth at temperatures between 35°C and 180°C. The points are measured values, the lines are curve fits using the ALI model. The isotherms for toluene at 35°C were measured with the flow-through method.

*Remark concerning Figure 3.6, acetone: For the acetone isotherms, only the measured values up to

a maximum temperature of 150°C were used for parameter fitting. The pronounced deviations observed in the diagram at 180°C (red diamonds) are presumably due to the decomposition of acetone by oxidation with the oxygen of the air. This leads to the formation of products which are better adsorbed, such as peroxides or acetic acid. It is altogether interesting and also of technical significance that it can already be recognised from the isotherm measurements whether and at what temperature decomposition of the solvent must be expected.

3.3.2 Measured Results for Ethyl acetate and Water

Figure 3.7 below compares the results of the measurements of the isotherm fields for ethyl acetate and water on activated carbon fibre cloth (ACC) and activated carbon granulate (GAC). The values measured for the activated carbon granulate (GAC1&GAC2) were taken from the literature [4, 5], and the measurements with the activated carbon fibre cloth (ACC2) refer to our own measurements with the equilibrium adsorption apparatus. The ALI model very well describes the isotherm fields for ethyl acetate, for the activated carbon granulate as well. The mean relative deviations between the calculated and the measured loadings are 6.1% for ACC2 and 2.1% for GAC1. GAC1 is a typical solvent recovery carbon with a high meso-pore fraction. Unfortunately, no measured values are available for gas concentrations of $<500\text{mg/m}^3$ for GAC1, so that the experimental verification of the Henry range remains to be investigated.

In Figure 3.7, it is also seen that for both ACC2 and GAC2 the water isotherm fields can be well described by the ALI model too. The mean relative deviations between the calculated and the measured loadings are ~13% for ACC2 and ~11% for GAC2. Considering the larger measurement errors in the extremely steep slope of the isotherms, roughly twice as large compared to the solvent measurements, these deviations are understandable.

Although, the prevailing academic opinion is, that at humidities above 40%_{rel.} the pore filling takes place by capillary condensation. This can apparently be described by an adsorption process as well. In [6], reference was made explicitly to the impossibility to distinguish thermodynamically between capillary condensation and multi-layer loading. From the behaviour of the water isotherms, based on the theory of capillary condensation and the Kelvin equation, we can derive conclusions about the pore size and pore size distribution. The very steep curve shows that ACC2 has a very narrow pore size distribution, i.e. only micro-pores. GAC2 has a somewhat greater average pore diameter indicated by the shift at the inflection points of the curves towards higher relative humidities. It also has a clearly wider pore size distribution indicated by the smaller slope. GAC2 is a relatively fine-

pored carbon which is used preferentially for the removal of VOCs at low concentrations rather than for solvent recovery.

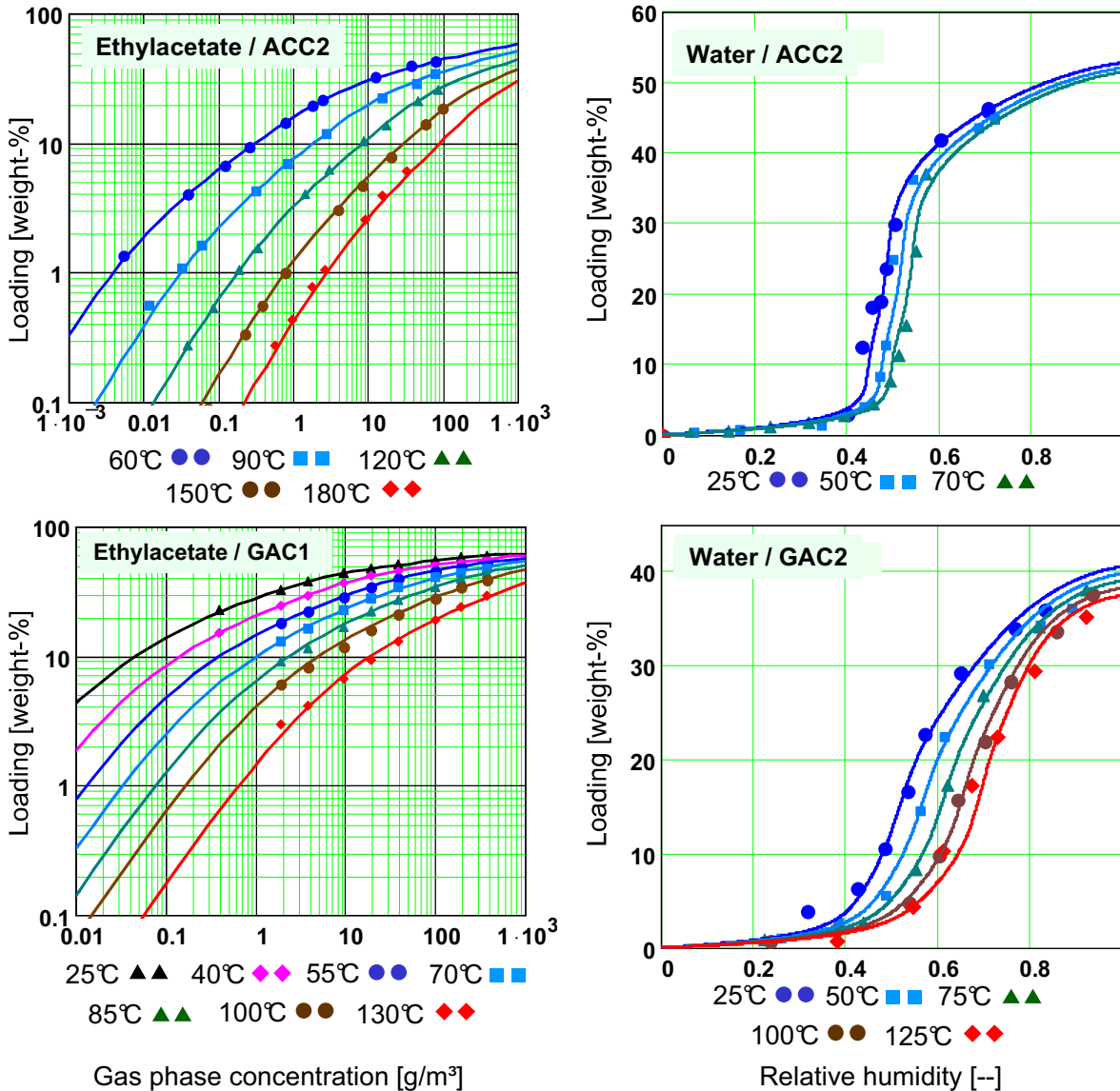


Figure 3.7: Comparison of the isotherm fields of ethyl acetate on ACC2 / GAC1 and water on ACC2 / GAC2. The points are measured values. The lines are curve fits using the ALI model.

4 Basic Principles of Condensation and Adsorption

4.1.1 Pore Filling Degree in Adsorption

For the description of the equilibrium vapour pressure p for the system adsorptive (a) plus adsorbent

(s), with two degrees of freedom, at a given temperature T as a function of a material composition, we have the possibility of using the mole fraction, mass fraction or e.g. the loading $X_a = \frac{m_a}{m_s} = \frac{\rho_a(T)}{\rho_s} = \rho_a(T) \cdot v_s$ between the limits 0 and 1. Thus, we could write e.g. $p = f(T, X_a)$.

However the parameters equilibrium vapour pressure p , temperature T and e.g. the loading X_a must be independent of each other. This is not possible here, because the density of the liquid adsorptive $\rho_a(T)$ is a function of temperature, but the density of the solid adsorbent, on the other hand, practically not, thus $\rho_s \neq f(T)$. Consequently, the mole fraction, the mass fraction and the loading are temperature-dependent. At a given volumetric loading, the lower the temperature the more substance is adsorbed in the pore. This considerably complicates comparisons of thermodynamic states, so that additional attention is required.

On the basis of the degree of pore filling Ξ , we can directly compare adsorption effects in pores of different sizes and at different temperatures. Decisive is how many molecules of the adsorptive (a) are bound with which binding energy to which energy-level-site in the pore. The degree of pore filling is therefore of greater physical meaning than the absolute amount of adsorptive in the pore. For further discussions and model development, the degree of pore filling Ξ therefore will be introduced as a measure of loading. It is defined in terms of the actual mass of the adsorptive m_a in the pores and the maximum possible mass of the adsorptive in the pores $m_{a,max}$, as

$$\Xi = \left(\frac{m_a}{\text{"Pore"}} \right) / \left(\frac{m_{a,max}}{\text{"Pore"}} \right) = \left(\frac{m_a}{m_s} \right) / \left(\frac{m_{a,max}}{m_s} \right) = \frac{m_a}{m_{a,max}} = \frac{n_a}{n_{a,max}} = \frac{X_{as}}{X_{as,max}} \quad (4.1)$$

The pore filling degree Ξ can have values between 0 and 1. Therefore it is obvious that all molar quantities are only in relation to the adsorptive (a) and not to the sum (a plus s) of the adsorptive (a) and adsorbent (s). The temperature dependence and the problematic fraction-oriented points of view, such as mole fraction or mass fraction, are therefore avoided. Measurements of the mass-specific maximum loading $X_{as,max}$ which decreases with increasing temperature, are described in [3] as a function of the temperature T .

4.1.2 Vapour Pressure Curve of an Adsorbate-Liquid

Formally, equation 4.2 for adsorption is identical with the equation for condensation, see [7], but includes the additional variable degree of pore filling Ξ . From this point of view, the adsorbate can be regarded as an unique and separate "adsorbate-liquid" for every degree of pore filling Ξ , with its own vapour pressure curve, and can be treated as such. In order to visualise this, points of the same degree of pore filling $\Xi = 0.3$ are plotted in the measured values for the isotherm fields, see Figure 4.1, for the solvent toluene and the vapour pressure curve derived from the "adsorbate-liquid" constructed. The points of constant degree of pore filling Ξ on the isotherms are referred to as isosteres. The isosteres are identical with the vapour pressure curves for the respective "adsorbate-liquid".

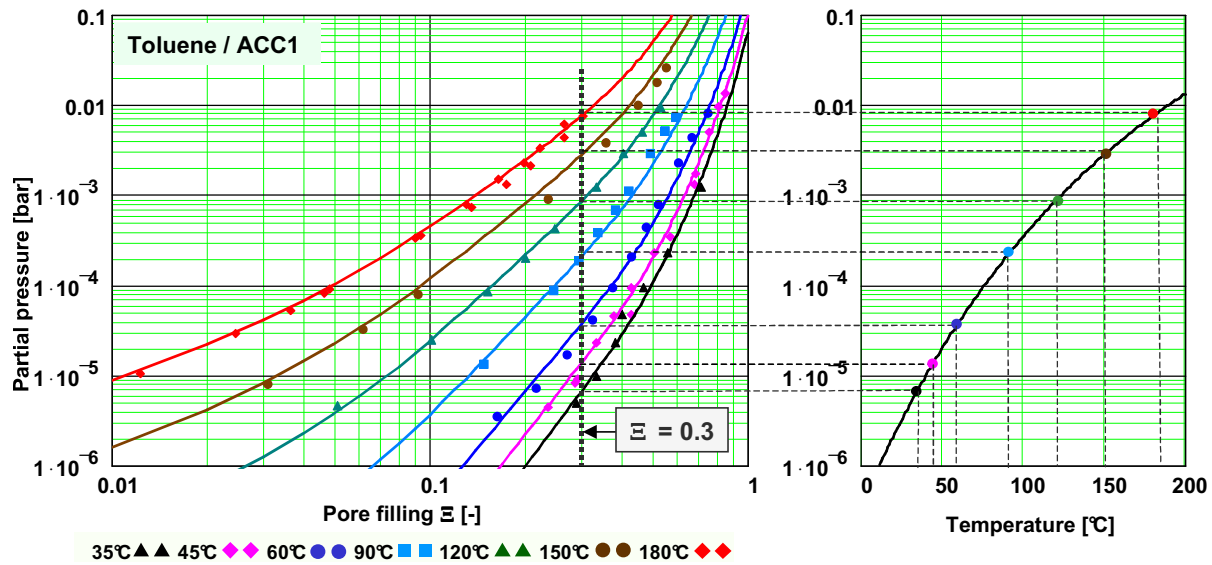


Figure 4.1: Adsorption isotherm field of toluene on ACC. The points are measured values, the lines are curve fits using the ALI model. For the pore filling ratio Ξ of 30% it is exemplarily shown, how the adsorbate-liquid vapour pressure curve results for $\Xi = 0.3$.

This allows us to thermodynamically treat the adsorption process entirely analogously to the condensation of clean materials. Using the degree of pore filling Ξ as a measure for adsorbent loading, the complete general vapour pressure equation for the "adsorbate-liquid" then becomes:

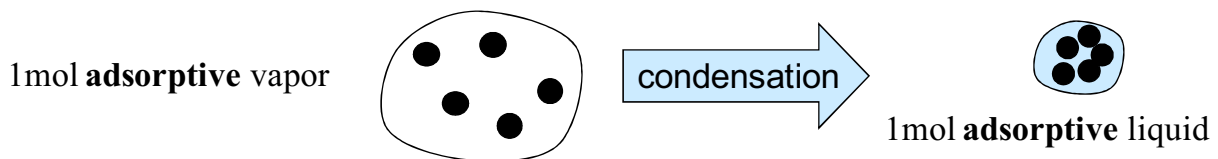
$$\ln\left(\frac{p(T, \Xi)}{p_{\text{std}}}\right) = \frac{\Delta H_{m\Xi, \text{ads}}(T, \Xi)}{R_m \cdot T} - \frac{\Delta S_{m\Xi, \text{ads}}^{\text{std}}(T, \Xi)}{R_m} \quad (4.2)$$

$\Delta H_{m\Xi, \text{ads}}(T)$ and $\Delta S_{m\Xi, \text{ads}}^{\text{std}}(T)$ are the temperature-dependent differential molar enthalpy of adsorption and the standard entropy of adsorption for the transition of the material from the gas phase to the adsorbed state, in relation to the standard pressure of 1bar in the gas phase for a constant degree of pore filling Ξ . At the same time, this equation is the general form of the adsorbate-liquid-isotherm (ALI) equation, because it is the implicit form of the function $\Xi = f(p, T)$, see [3].

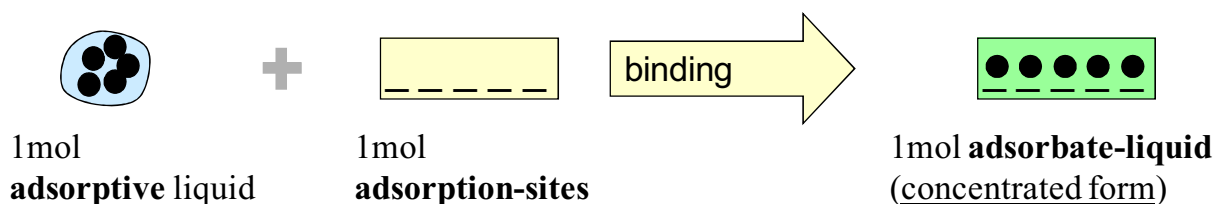
5 Application of the ALI Model Parameters

The adsorbate-solvent-isotherm (ALI) equations enables the thermodynamically consistent description of the measured adsorption results for the adsorptives toluene, n-pentane, n-octane, propanol-2, acetone, isobutyl glycol ether acetate, ethyl acetate and water on micro-porous activated carbon fibre cloth and micro-pore and meso-pore activated carbon granulates over the range of measured temperatures from 35°C to 180°C, with gas loading ~5mg/m³ to ~200,000mg/m³. For this description, the adsorption process was divided into three separate steps, see [7]:

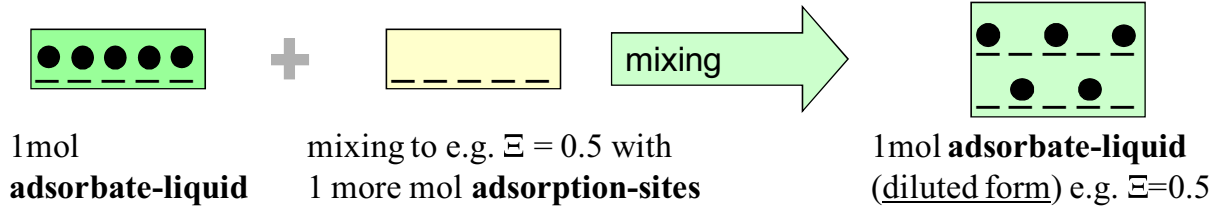
1. Condensation of the gas-phase adsorptive to the liquid phase at the temperature T



2. Binding of the liquid adsorptive to the non-occupied adsorption positions, adsorption-sites, i.e. formation of the "adsorbate-liquid" in its concentrated form at the temperature T.



3. Uniform distribution of the adsorbed adsorptive with its molar volume on the adsorbent to its final molar volume on the adsorbent. It is a mixing or a dilution of the adsorbate-liquid from its concentrated form to its final diluted form by the factor $1/\Xi$ at the temperature T .



From the equilibrium vapour pressure $p_0(T)$ of the pure liquid adsorptive at the temperature T and the model parameters, the ALI equations for the equilibrium vapour pressure $p(T, \Xi)$ of the adsorbate-liquid follow:

$$\ln\left(\frac{p(T, \Xi)}{p_{\text{std}}}\right) = \frac{\Delta H_{\text{m,con}}(T) + \Delta H_{\text{m}\Xi, \text{bin}}(\Xi)}{R_m \cdot T} - \frac{\Delta S_{\text{m,con}}^{\text{std}}(T) + \Delta S_{\text{m}\Xi, \text{bin}}(\Xi) + \Delta S_{\text{m}\Xi, \text{mix}}(\Xi)}{R_m} \quad (5.1)$$

The terms on the right side express the molar enthalpy of condensation $\Delta H_{\text{m,con}}(T)$, the molar differential bond enthalpy $\Delta H_{\text{m}\Xi, \text{bin}}(\Xi)$, the molar standard entropy of condensation relative to 1bar $\Delta S_{\text{m,con}}^{\text{std}}(T)$, the molar differential bond entropy $\Delta S_{\text{m}\Xi, \text{bin}}(\Xi)$ and the molar differential mixture entropy $\Delta S_{\text{m}\Xi, \text{mix}}(\Xi)$.

The both terms $\Delta H_{\text{m,con}}(T)$ and $\Delta S_{\text{m,con}}^{\text{std}}(T)$ can be derived from literature. The following two equations

$$\Delta H_{\text{m}\Xi, \text{bin}}(\Xi) = \Delta H_{\text{lin}} \cdot (1 - \Xi) + \Delta H_{\text{exp}} \cdot e^{\frac{-k_{\text{b,ex}} \cdot \Xi}{(1-\Xi)}} \quad (5.2)$$

$$\Delta S_{\text{m}\Xi, \text{bin}}(\Xi) = \Delta S_{\text{lin}} \cdot (1 - \Xi) + \Delta S_{\text{exp}} \cdot e^{\frac{-k_{\text{s,ex}} \cdot \Xi}{(1-\Xi)}} \quad (5.3)$$

allow the application of the “Monte-Carlo”-fitting-procedure, resulting in the six fitting-parameters

and finally our own new developed entropic-equation, see [7]

$$\Delta S_{m\Xi, \text{mix}}(\Xi) = \Xi \cdot (1 - \Xi)^{\frac{1-\Xi}{\Xi}} \quad (5.4)$$

5.1 Calculation of the Adsorbate-Liquid-Isotherm Fields

Table 5.1 presents the relevant parameters for application of the ALI model with the above equations for the eight solvents under investigation. These are the two adapted material parameters, the specific pore volume v_s of the adsorbent and the relative temperature coefficient for the density α_{as} of the adsorptive, plus the six fit parameters of the ALI model ΔH_{lin} , ΔH_{exp} , $k_{h,ex}$, ΔS_{lin} , ΔS_{exp} and $k_{s,ex}$. The user is then able to calculate the isotherm fields with the simplest means over the entire pore filling degrees and temperatures close to the critical temperature or apply the equations in design programs for the dimensioning of apparatus, systems and devices.

	v_s [ml/100g]	$-\Delta H_{lin}$ [kJ/mol]	$-\Delta H_{exp}$ [kJ/mol]	$k_{h,ex}$ [-]	$-\Delta S_{lin}$ [J/mol/K]	$-\Delta S_{exp}$ [J/mol/K]	$-k_{s,ex}$ [-]	$-\alpha_{as}$ [1/K] $\times 10^{-3}$
Toluene / ACC1	52.0	30.1	29.3	9.4	15.5	51.0	8.7	0.19
n-Pentane / ACC1	48.0	37.0	11.8	24.7	36.0	20.5	27.3	0.18
n-Oktane / ACC1	47.9	45.2	7.2	20.3	18.3	14.0	36.9	0.86
Propanole-2 / ACC1	43.8	25.2	-10.9	20.6	29.6	-46.3	22.1	0.29
Acetone / ACC1	54.0	17.9	11.2	20.2	8.1	19.2	22.4	0.22
i-Butyl glykol ether- acetat / ACC1	50.8	31.2	-2.3	25.2	-45.9	52.2	1.0	0.52
Ethyl acetate / ACC2	69.0	31.2	6.2	9.9	28.6	13.2	3.9	0.03
Ethyl acetate / GAC1	67.8	55.5	-32.2	1.4	90.8	-76.6	1.6	0.55
Water / ACC2	52.8	5.4	-3.4	1.5	24.1	13.0	8.7	0.57
Water / GAC2	40.6	4.9	-2.6	3.0	29.0	9.4	13.3	0.76

Table 5.1: Parameters from the measurement value fitting procedure to be used in the ALI equation. The parameters are valid up to temperatures of 180°C, for acetone only up to 150°C, see Figure 3.6 for reason.

6 Summary

For the solvents toluene, pentane, n-octane, propanol-2, acetone, isobutyl glycol ether acetate, ethyl acetate and water, the partial vapour pressure was measured as a function of temperature and degree

of pore filling for adsorption on activated carbon fibre cloth and the results were presented. In order to understand the results, to allow extrapolations and interpolations, and to make them accessible for calculations, an adsorbate-liquid-isotherm (ALI) model was developed, which is thermodynamically consistent and includes the isotherms of Langmuir and Dubinin-Asthakov. Using a Monte Carlo method, curve fit parameters were calculated for the differential molar binding enthalpy and the differential molar binding entropy in a multi-step procedure. This allows extrapolations virtually to any arbitrary region of low gas concentration with certainty, as the ALI equation passes over to a Henry isotherm for low adsorbent loadings and correctly describes the temperature dependence of the isotherms. Such regions are at present practically inaccessible for measurements with a reasonable effort, if at all. Furthermore, for solvents with high boiling points it is possible on the basis of measurements at higher temperatures, e.g. more than 150°C, to reliably extrapolate to isotherms at room temperature.

7 Appendix

7.1.1 Acknowledgements

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7.1.2 Nomenclature

Designation	Symbol	Unit
moles of component i	n_i	mol
mass of component i	m_i	kg

mass fraction	$\xi_i = \frac{m_i}{m}$	-
mass loading of component j by component i	$X_{ij} = \frac{m_i}{m_j}, X_{ij,max} = \frac{m_{i,max}}{m_j}$	g/100g
pore filling degree $\Xi \neq f(j)$	$\Xi = \frac{X_{ij}}{X_{ij,max}}$	-
concentration	C	g/m_N^3
temperature, absolute	T	K
volume	V	m_N^3
specific pore volume	v_s	ml/100g
partial pressure of component i	p_i	bar
vapour pressure of the pure component	p_0	bar
standard reference pressure	$p_{std} = p_{Standard} = 1\text{bar}$	$10^5 \cdot \frac{\text{N}}{\text{m}^2} = 1\text{bar}$
general molar gas constant	R_m	$8.314 \frac{\text{J}}{\text{mol}\cdot\text{K}}$
differential, molar enthalpy difference wrt Ξ	$\Delta H_{m\Xi}$	J/mol
differential, molar entropy difference wrt Ξ	$\Delta S_{m\Xi}$	J/(mol·K)

7.1.3 Indices

Designation	Symbol
molar, differential wrt Ξ	$m\Xi$
adsorptive (gas- or liquid-phase)	,a
adsorbent	,s
adsorbate	,as
standard	,std
with reference to adsorption	,ads
curve fitting parameter, linear	,lin
curve fitting parameter, exponential	,exp
curve fitting parameter, exponential relative to H	h.ex
curve fitting parameter, exponential relative to S	s.ex

7.1.4 Abbreviations

Designation	Symbol
activated carbon fibre cloth, Chemviron,type FM5/250	ACC_1
activated carbon fibre cloth, Kynol, type 5092-15	ACC_2
activated carbon granulate, Degussa, type WSIV	GAC_1
activated carbon granulate, Calgon Carbon Corp.,type BPL	GAC_2

7.1.5 Literature

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