APPNOTE **1-4**

The Use of Mixture and Pure Gas Adsorption Isotherms for Further Calculations and Predictions

3P INSTRUMENTS

Characterization of
particles • powders • pores

3P INSTRUMENTS offers two general ways to obtain information about mixed gas adsorption processes; first with the measurement of the dynamic sorption process with the **mixSorb L** by 3P INSTRUMENTS and second by use of the **3P sim** software of the **mixSorb L** to calculate mixed gas data using pure gas isotherms. The **mixSorb L** offers the tools not only to measure the mixed gas isotherms in practice, but also to compare the results with various theories to include specific effects of the adsorption processes on the porous materials investigated. The 3P sim software provides the ability to predict mixture equilibrium data by well-established models **(Table 1)**. The 3P sim simulation software also provides the tools to estimate parameters for mixed gas separation processes such as the saturation capacity, the affinity constant, and the Sips exponent as well as the temperature dependencies of each.

Table 1: *Models to Predict Mixture Equilibrium Data from Pure Component Isotherms Provided by 3P-Sim*

Isotherm model	Maximal number of components provided by 3P sim	Remarks
IAST with Langmuir [1]	4	Solved by an iterative method for root determination
IAST with Toth [2]	4	Solved by Newton's method
Multi component Langmuir (Markham and Benton) [3]	4	Simple, analytical solution
Multi-Component Sips [4]	4	Simplified equation, Simple, analytical solution
Multi-Component Dualsite Langmuir [5]	4	Simple, analytical solution
IAST with Dualsite Langmuir [5]	4	Solved by Newton's method

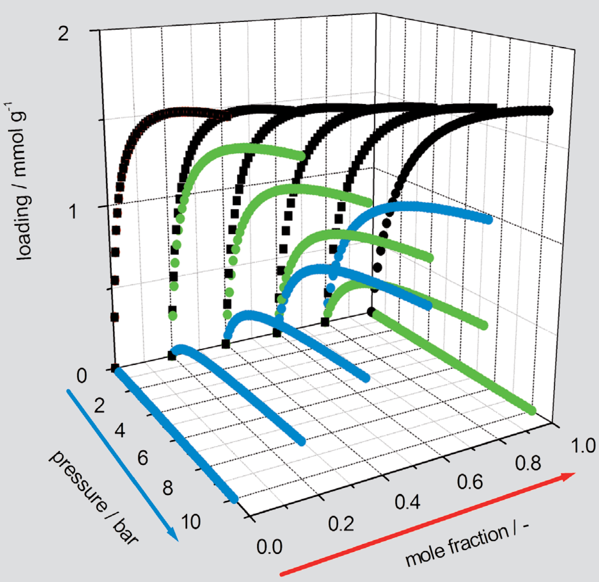

Figure 1: *Illustration of different calculations with mixture models using a 3D-plot (black: total loading, green: partial loading component A, blue: partial loading component B, blue labelling: calculation with constant gas phase composition, red labelling: calculation with constant total pressure)*

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Experimental

For this study, gas adsorption isotherms were measured with a high pressure sorption devised at different temperatures. The isotherms are shown in **Figure 2** for methane and **Figure 3** for carbon dioxide.

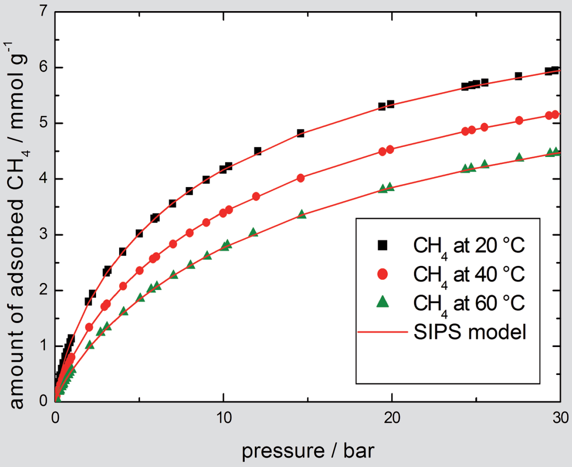

Figure 2: *Methane isotherms on activated carbon A for determination of isotherm parameters, measured with a high pressure sorption device. Fits are calculated data with Sips parameters from* ***Table 2****.*

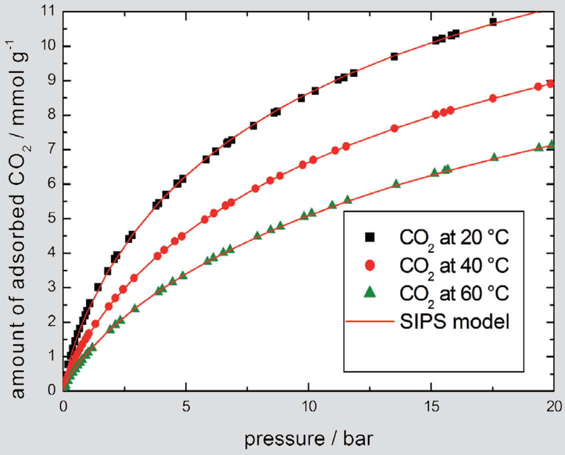

Figure 3: *Carbon dioxide isotherms on activated carbon A for determination of isotherm parameters, measured with a high pressure sorption device. Fits are calculated data with Sips parameters from* ***Table 2****.*

Results

The isotherm parameters listed in **Table 2** were determined from the equilibrium data by use of the 3P sim software package.

Table 2: *Sips parameters calculated from Isotherms using 3P sim Software*

Isotherm parameter	Values for CH_4	Values for CO_2
Saturation capacity at 20 °C	8.561 mmol g^{-1}	18.353 mmol g^{-1}
Affinity constant at 20 °C	0.09386 bar $^{-1}$	0.0862 bar $^{-1}$
Sips exponent at 20 °C	0.79614	0.7874
Temp. dependency of affinity constant	10.7 kJ mol^{-1}	15.7 kJ mol^{-1}
Temp. dependency of saturation capacity	1.181	1.228
Temp. dependency of Sips-exponent	0.4824	0.0642

By applying these isotherm parameters and calculations for non-isothermal conditions, the breakthrough behavior can be described with the 3P sim software package as seen in **Figure 4**.

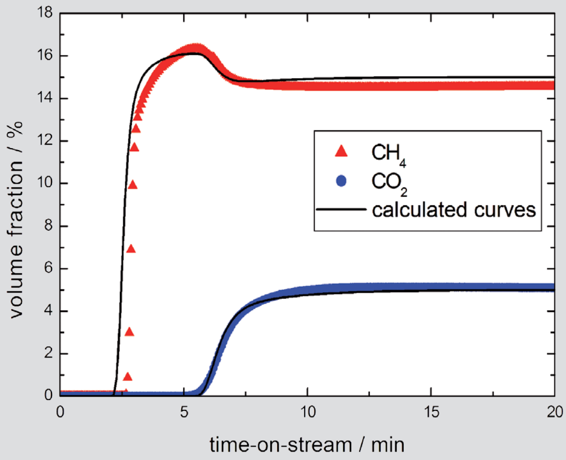

Figure 4: *Measured breakthrough curves for 15% methane and 5% carbon dioxide in helium and the calculated curves based on multi component Sips-model.*

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From the fitting of the measured breakthrough curves, a linear driving force constant (LDF-value [3]) was determined to be 12 min^{-1} for methane and 9 min^{-1} for carbon dioxide for the activated carbon A under experimental conditions. Due to the similar LDFvalues for methane and carbon dioxide, it can be concluded that the measured separation effect is based on the different sorption capacities of both adsorptives and that there are no relevant steric kinetic separation effects on this material.

Conclusion

Separation effects can be determined by measurement of the breakthrough curves of gas mixtures in a carrier gas using the **mixSorb L**. With the combination of the pure gas isotherms and their corresponding breakthrough curves along with data fitting using a dynamic model, LDF-constants can be estimated for further parametric studies to predict the source of the separation effect. It is possible to investigate adsorbents and their separation performance under real-world conditions using the dynamic method under lab conditions. Similar LDF-values from the **3P sim** calculation shows that a separation effect is based on the difference in sorption capacities of both adsorptives and not on steric-kinetic separation effects.

References

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