3P sim

mixSorb
Dynamic Sorption Analyzer

A modeling and evaluation tool for dynamic sorption data

TOOLS FOR DISCOVERY

3P
INSTRUMENTS

Characterization of
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3P sim

**A modeling and evaluation tool
for dynamic sorption data**

Introduction

Modeling of dynamic sorption proces-ses are very useful for the understand-ing of sorption characteristics on fixed bed adsorbers. With the help of such tools, the experimental time can be dras-tically reduced and parametric studies can be easily performed. The simula-tion and evaluation tool **3P sim** is pro-vided with the new dynamic sorption analyzer series "mixSorb" for the inves-tigation of breakthrough characteristics.

This software allows the calculation of equilibrium data of mixtures from pure component isotherms as well as the evaluation of breakthrough curves, based on mass- and energy balances. The available solver is easy to handle and can be operated by untrained ope-rators. As an example, the calculation of CH_4 / CO_2 breakthrough curves on acti-vated carbon is shown.

Gas Purification and Separation
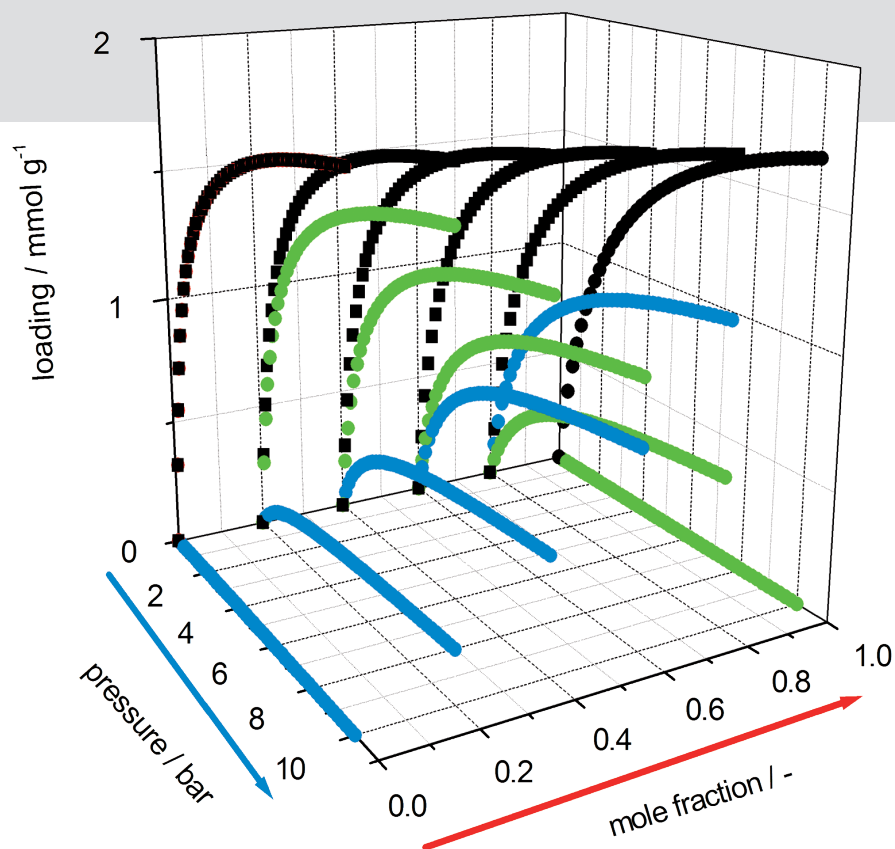
Figure:
Different calculations with mixture models using a 3D-plot
black: total loading
green: partial loading component A
blue: partial loading component B
blue labelling: calculation with constant gas phase composition
red labelling: calculation with constant total pressure

Data Flow

Pure Component Isotherms

Equilibrium Data and Breakthrough Curves

3P sim

Isotherm Fitting

With **3P sim** measured isotherm data can be fitted with the following mathematical isotherm models:

- HENRY
- LANGMUIR
- TOTH
- SIPS
- FREUNDLICH
- DUALSITE LANGMUIR
- DUALSITE LANGMUIR SIPS

Prediction of Mixture Equilibria

The program allows the calculation of total and partial loadings at given pressures or compositions and supports the following theories:

- IAST* with LANGMUIR
- IAST with TOTH
- IAST with DUALSITE LANGMUIR
- IAST with DUALS. LANGMUIR SIPS
- Multicomponent LANGMUIR
- Multicomponent SIPS

* Ideal Adsorption Solution Theory

Dynamic Simulation

- **3P sim** provides solutions for mass- and energy balances which allow simulations without user precognition or programming skills.
- Technically relevant transport parameters (e.g., LDF* constants) are accessible
- Simulation of breakthrough curves and temperature profiles

* Linear Driving Force
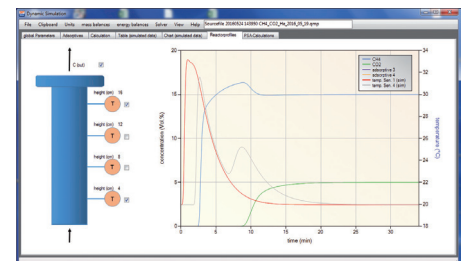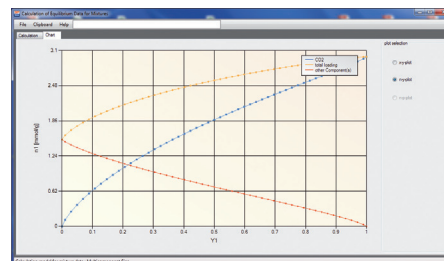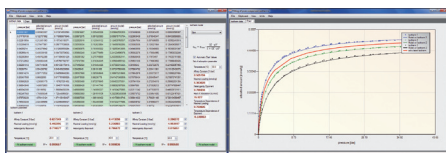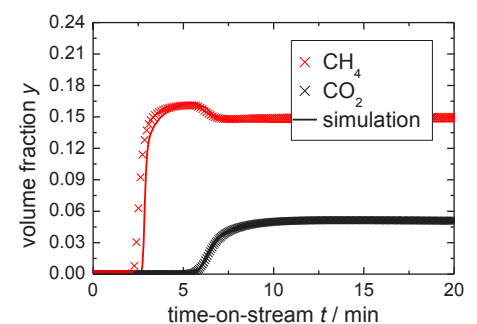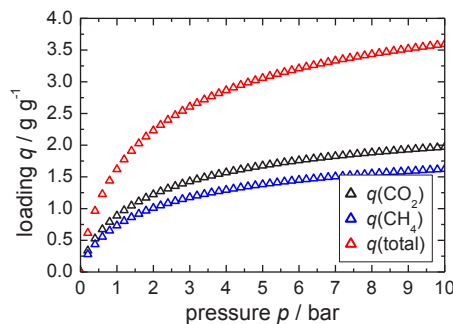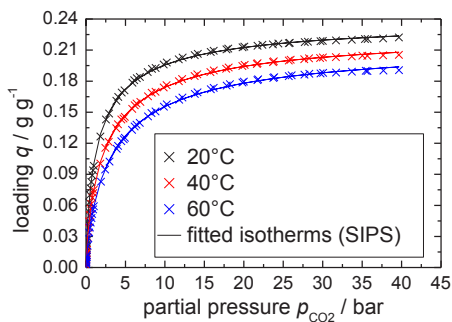
Mathematical description of the Isotherms for further calculation. With a set of measured isotherms, the temperature dependence can be calculated and a theoretical interpolated isotherm at a given temperature can be predicted.

Mixture equilibria can be implemented in Dynamic Simulations.

Complete data set for **parametric studies.**

Conclusion

By measuring breakthrough curves of mixtures in a carrier gas, separation effects can be observed. If the isotherms are well known, a fitting of such breakthrough curves with a dynamic model is possible to get information for further parametric studies. With the dynamic method, it is possible to investigate adsorbents regarding their separation performance under relevant conditions. Such valuable performance characteristics can only be derived from dynamic experiments. **3P sim** allows parametric studies to reduce experimental effort and improves the understanding of separation processes.

mixSorb
Dynamic Sorption Analyzer

Dynamic Sorption Analyzer

Industrial adsorbents such as active carbons, zeolites and silica gels are widely used in adsorptive separation processes on a multi-ton scale. The after-treatment of exhaust gasses, the removal of carbon dioxide in bio gas plants, purification and fractionation of natural gas, air separation, respiratory protection and separation of isomers are just a few examples where adsorptive separation is employed as the most efficient and economic separation technique.

Specifications

World-class performance is ensured by designing to very stringent instrument specifications thus ensuring the highest quality data.
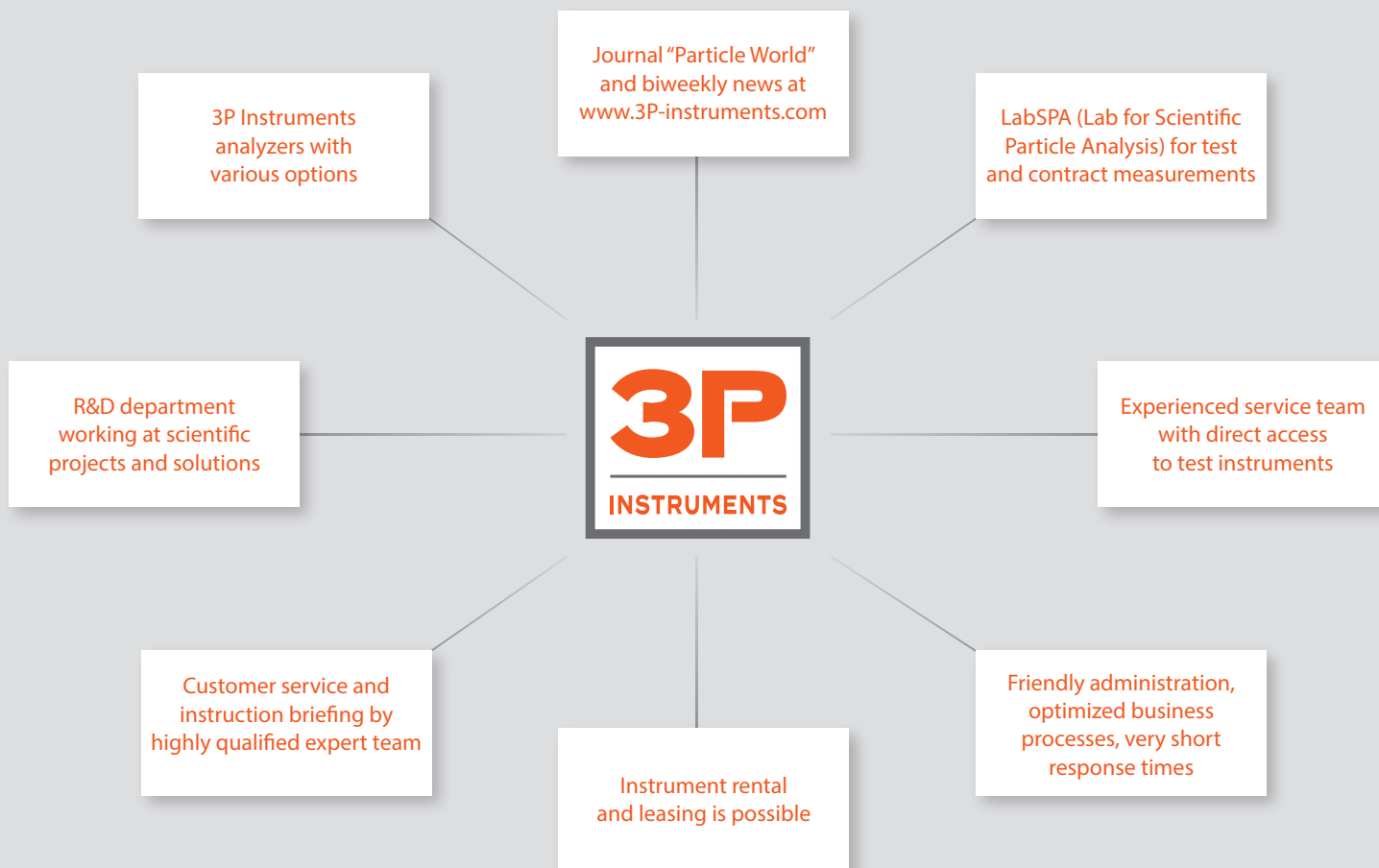
Adsorber:	1
No. of Mass Flow Controllers*:	Up to 4
Max. Pressure:	Up to 68 bar
Sample Preparation:	In-situ
Temperature Range:	-20 – 400 °C
Height:	960 mm (38 in)
Width:	860 mm (34 in)
Depth:	640 mm (25 in)
Weight:	120 kg (265 lbs)

* Mass flow controllers are available in different ranges. For optimal instrument configuration with respect to customer's needs.

Features and Benefits

- **Large Flow Range**

  Investigation of mixture equilibrium and kinetics, downscaling of technical processes.

- **Built-in Thermal Conductivity Detector (TCD)**

  Automated time-resolved measurement of outlet gas composition.

- **Built-in Sample Preparation up to 400°C**

  Investigation of hydrophilic materials (i.e., zeolites and silica gels).

- **Automated Pressure Regulation**

  Completely programmable for operator-free performing of pressure steps.

- **Automated Gas and Vapor Mixing**

  No need of multiple pre-mixed gas tanks, increasing of flexibility of measurement conditions.

- **Optional Gas Analysis via Interfaced MS**

  Investigation of ternary and more complex systems.

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with direct access
to test instruments

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instruction briefing by
highly qualified expert team

Instrument rental
and leasing is possible

Friendly administration,
optimized business
processes, very short
response times

www.dynamicsorption.com

collects and summarizes all the features, advantages, examples
and knowledge of dynamic sorption (or flow sorption) methods.
Feel free to browse through the pages about breakthrough
curves, mixture adsorption and the commercial breakthrough
analyzers of the mixSorb series, and our specialist literature
for download under "Resources".