



dynaSim[™]
a modeling and evaluation tool for
dynamic sorption data

Characterizing Today's Materials — Discovering Tomorrow's[™]



Tools for Discovery

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Dynamic Flow Sorption

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dynaSim™

a modeling and evaluation tool
for dynamic sorption data

Introduction

Modeling of dynamic sorption processes are very useful for the understanding of sorption characteristics on fixed bed adsorbers. With the help of such tools the experimental time can be drastically reduced and parametric studies can be easily performed. The simulation and evaluation tool **dynaSim™** is provided with the new dynamic sorption analyzer **dynaSorb BT™** for the investigation 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 operators. As an example, the calculation of CH₄ / CO₂ breakthrough curves on activated carbon is shown.

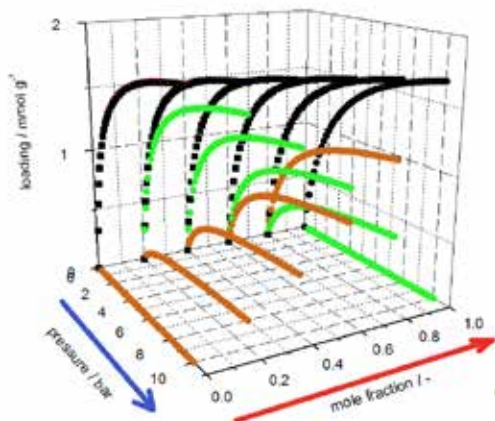


Illustration of different calculations with mixture models using a 3D-plot (black: total loading, green: partial loading component A, brown: partial loading component B, blue labeling: calculation with constant gas phase composition, red labeling: calculation with constant total pressure)

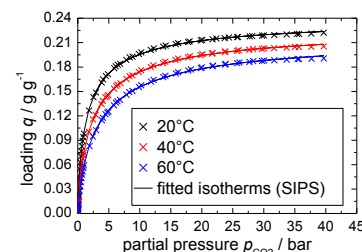
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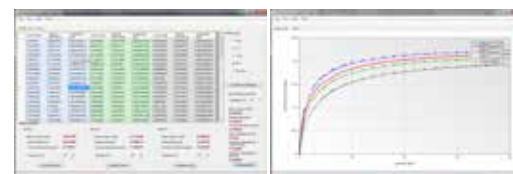
Isotherm Fitting

With **dynaSim™**, measured isotherm data can be fitted with the following mathematical isotherm models:

- HENRY
- LANGMUIR
- TOTM
- SIPS
- FREUNDLICH



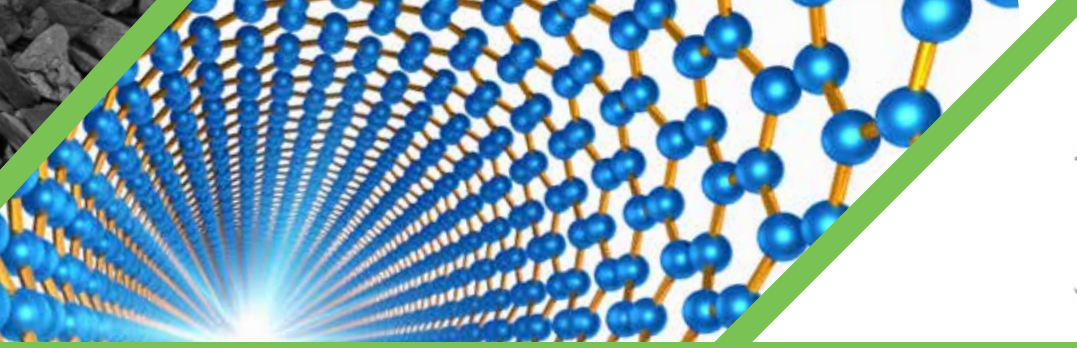
With a set of measured isotherms, the **temperature dependence** can be calculated and a theoretical interpolated isotherm at a given temperature can be **predicted**.



→ **Mathematical** description of the Isotherms can be used for calculation of **mixture equilibria** and **Dynamic Simulations**.

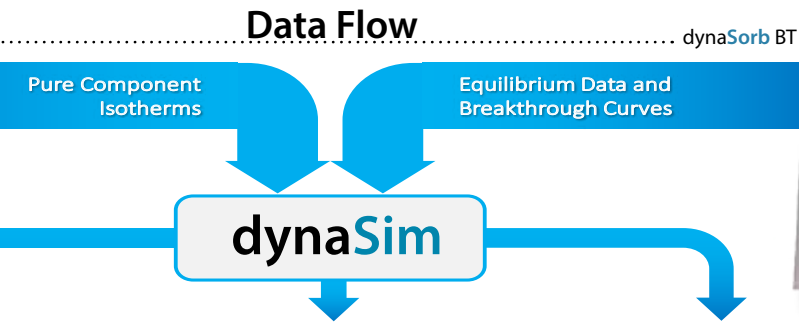


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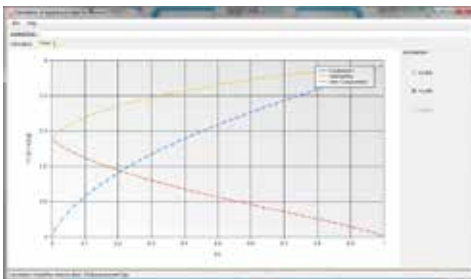
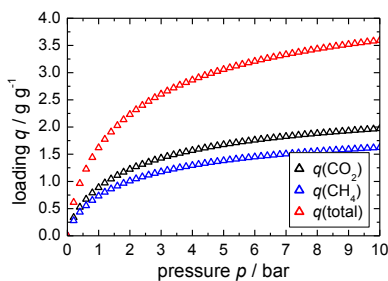
Dynamic Flow Sorption



Prediction of Mixture Equilibria

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

- IAST* with LANGMUIR
- IAST with TOTH
- Multicomponent LANGMUIR
- Multicomponent SIPS

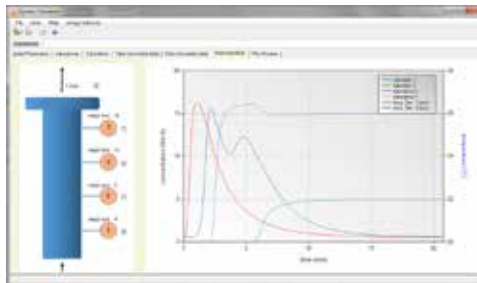
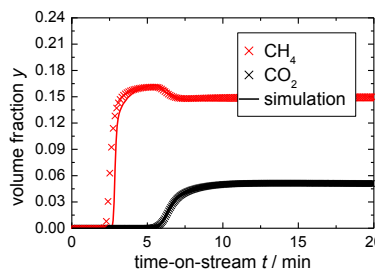


→ Mixture equilibria can be implemented in Dynamic Simulations.

*Ideal Adsorption Solution Theory

Dynamic Simulation

- **dynaSim™** provides solvers 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



→ Complete data set for **parametric studies**.

*Linear Driving Force

Conclusion

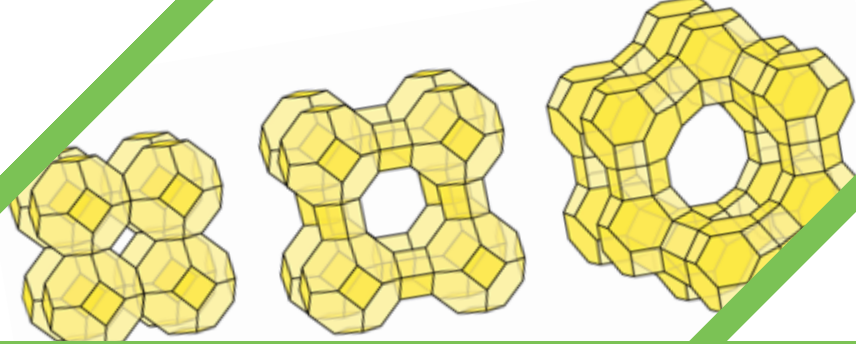
By measuring breakthrough curves of mixtures in a carrier gas, separation effects can be observed. If the isotherms are well known, fitting of such breakthrough curves with a dynamic model is possible to get information for further parametric studies. With the dynamic method, it is possible to investigate adsorbents regarding their separation performance under relevant conditions.

Such valuable performance characteristics can only be derived from dynamic experiments. **dynaSim™** allows parametric studies to reduce experimental effort and improves the understanding of separation processes.

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Dynamic Sorption Breakthrough 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.

Visit www.quantachrome.com for more detailed instrument specifications and downloadable brochures.



Features & 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 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.

Specifications

World-class performance is ensured by designing to very stringent instrument specifications thus ensuring the highest quality data.

Adsorber:	1
Number of Mass Flow Controllers ¹ :	2 Standard, 3 or 4 Optional
Max. Pressure [bar]:	10
Sample Preparation:	In-situ
Temperature Range Heating Mantle:	Ambient to 400°C
Temperature Range Circulator Bath:	-20° to 90°C
Height:	80 cm (31.5 in)
Width:	95 cm (37.5 in)
Depth:	60 cm (23.5 in)
Weight (approximate):	200 kg (440 lbs)

¹Mass flow controllers are available in different ranges (0.1, 0.2, 0.5, 1, 2, 5, 10, 20 L/min) for optimal instrument configuration with respect to customer's needs.

