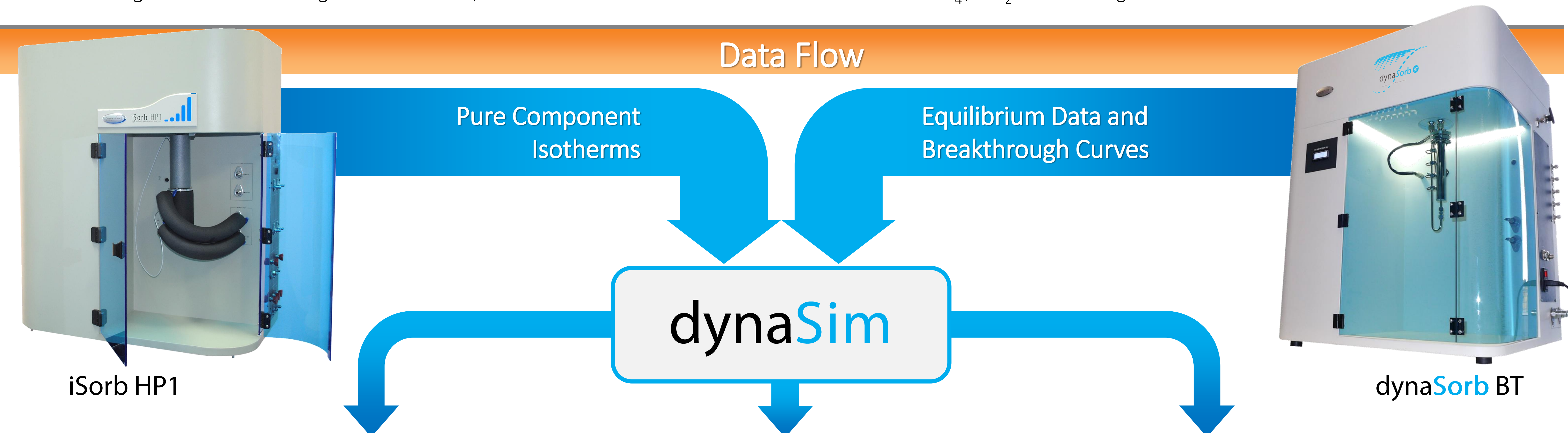




Introduction

Modeling of dynamic sorption processes is very useful for the understanding of sorption characteristics on fixed bed adsorbents. With the help of such tools, the experimental time can be drastically reduced and parametric studies can be easily performed. Within the package of the new dynamic sorption analyzer **dynaSorb BT** for the investigation of breakthrough characteristics, the simulation and evaluation

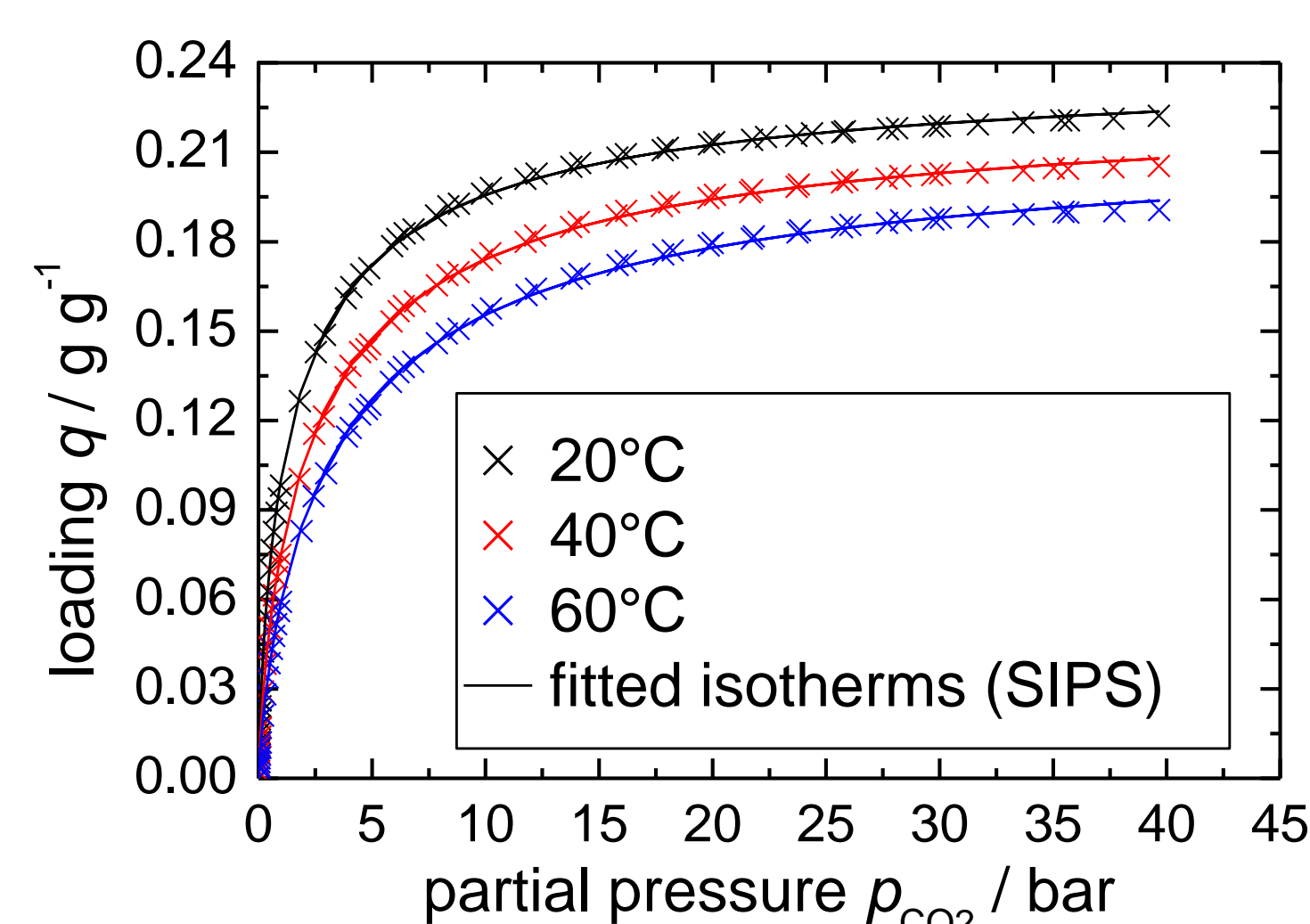
tool **dynaSim** is provided. This software allows the calculation of equilibrium data of mixtures from pure component isotherms, as well as the evaluation of breakthrough curves, based on mass- and energy balances. The available solver is easy to handle and can also be operated by untrained operators. As an example, the calculation of CH₄/CO₂ breakthrough curves in He on activated carbon is shown.



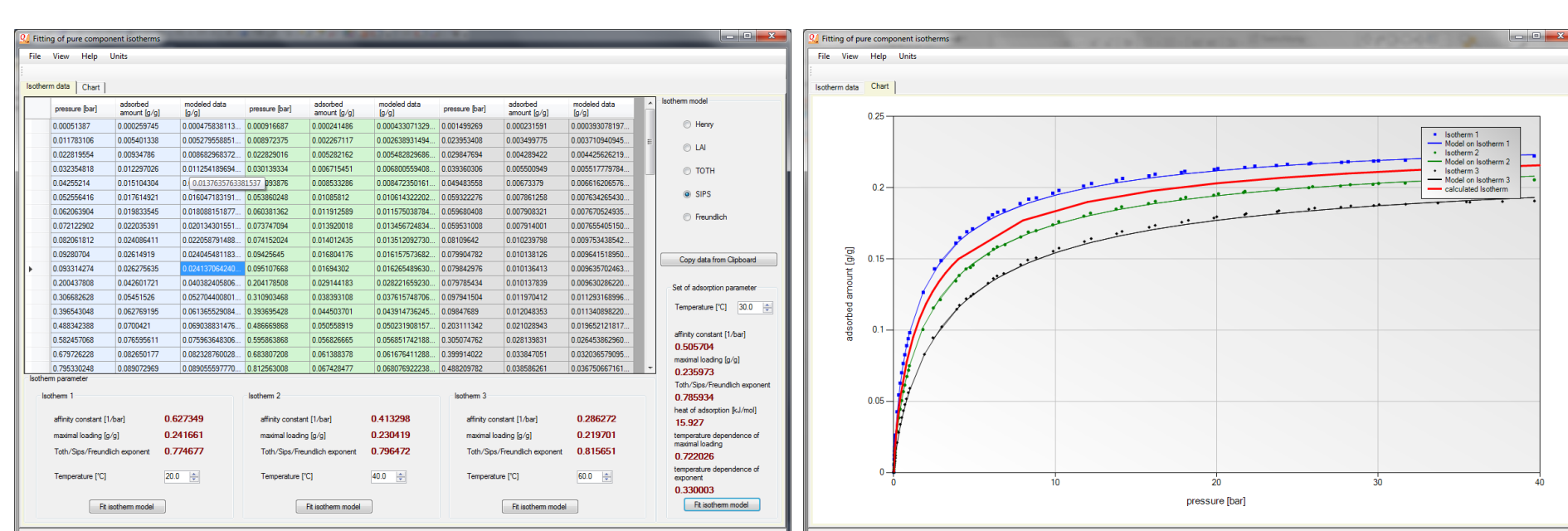
Isotherm Fitting

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

- HENRY
- LANGMUIR
- TOTH
- 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.

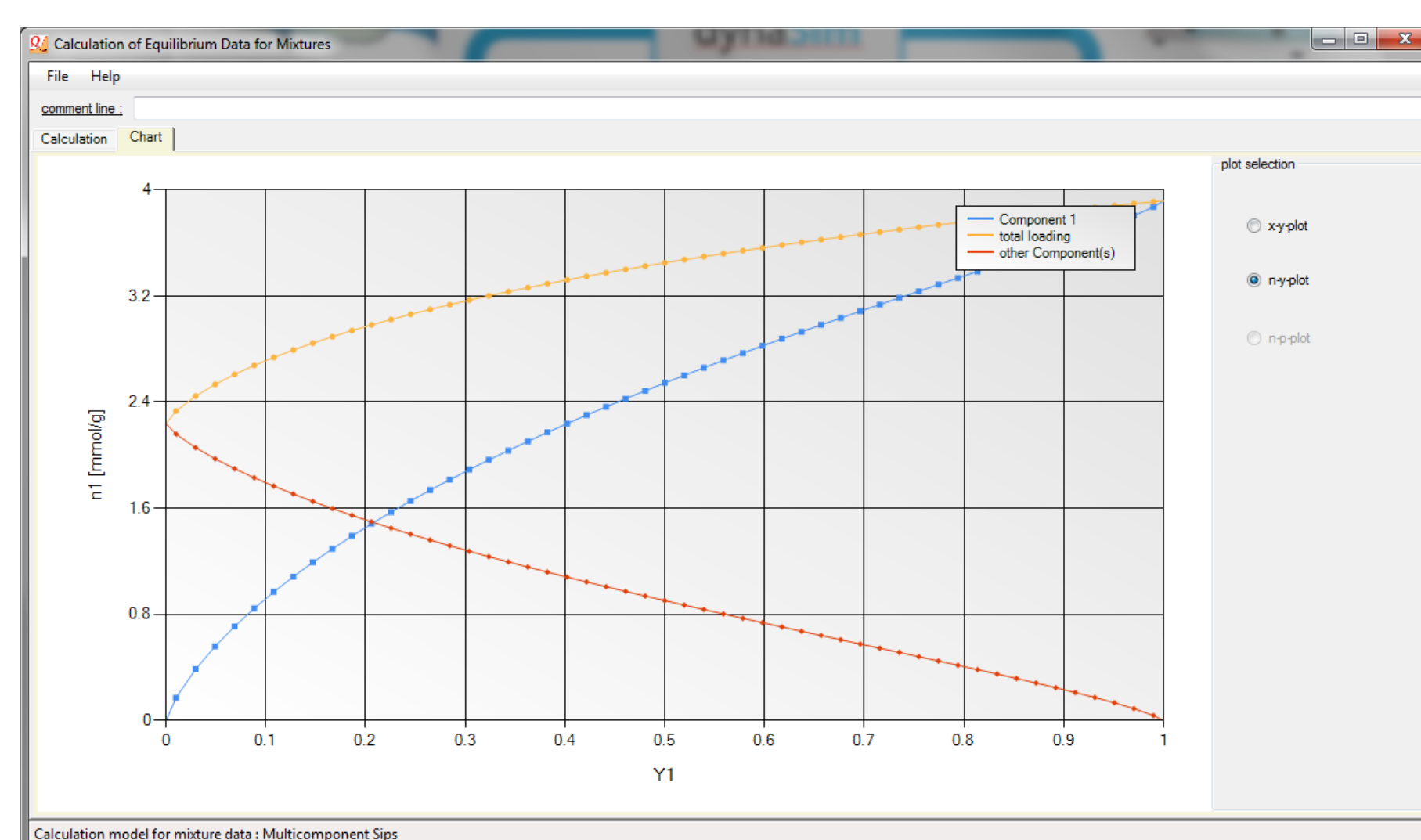
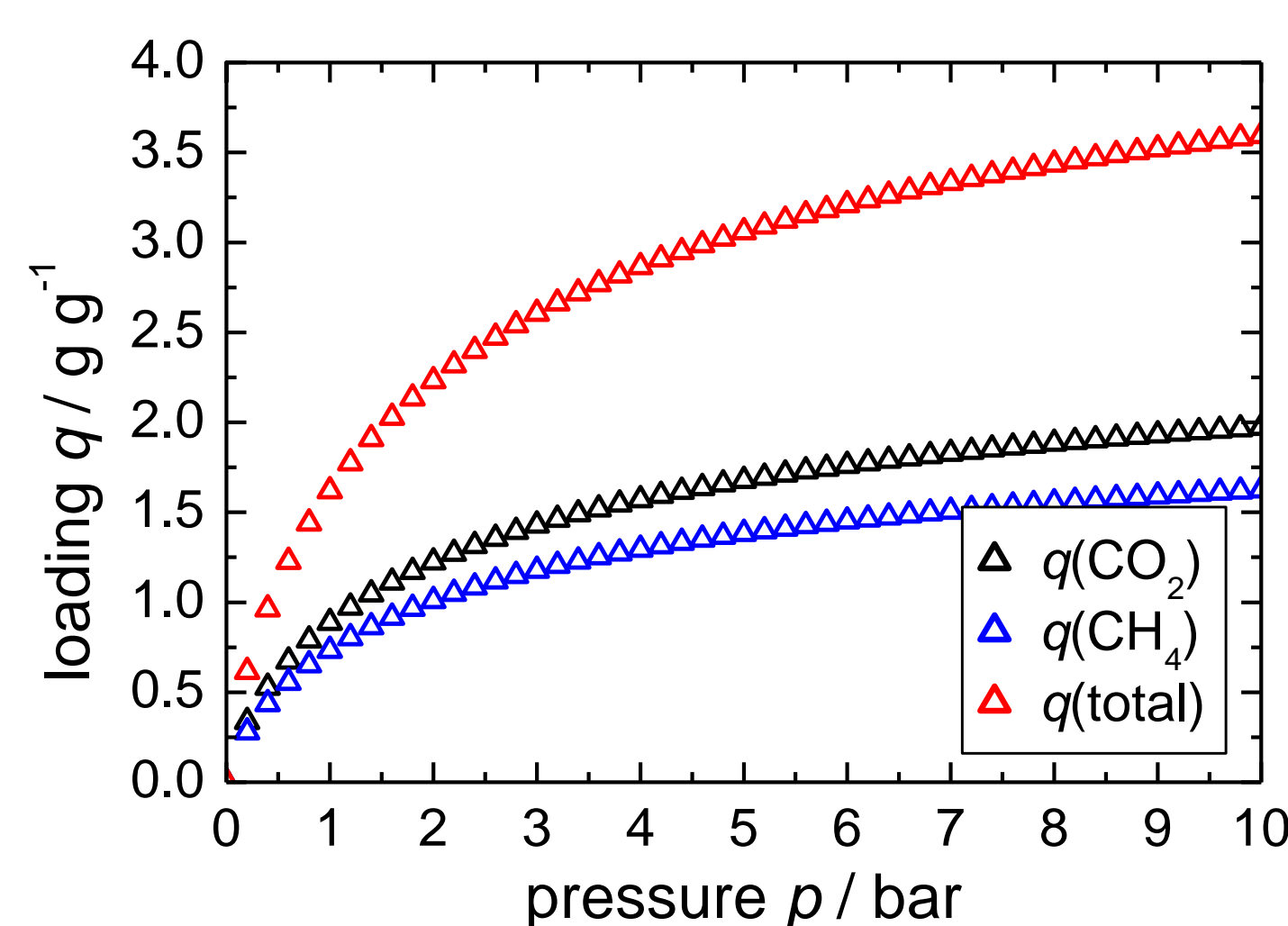


→ **Mathematical description** of the Isotherms can be used for calculation of **Mixture Equilibria** and **Dynamic Simulations**.

Prediction of Mixture Equilibria

The program allows calculations 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

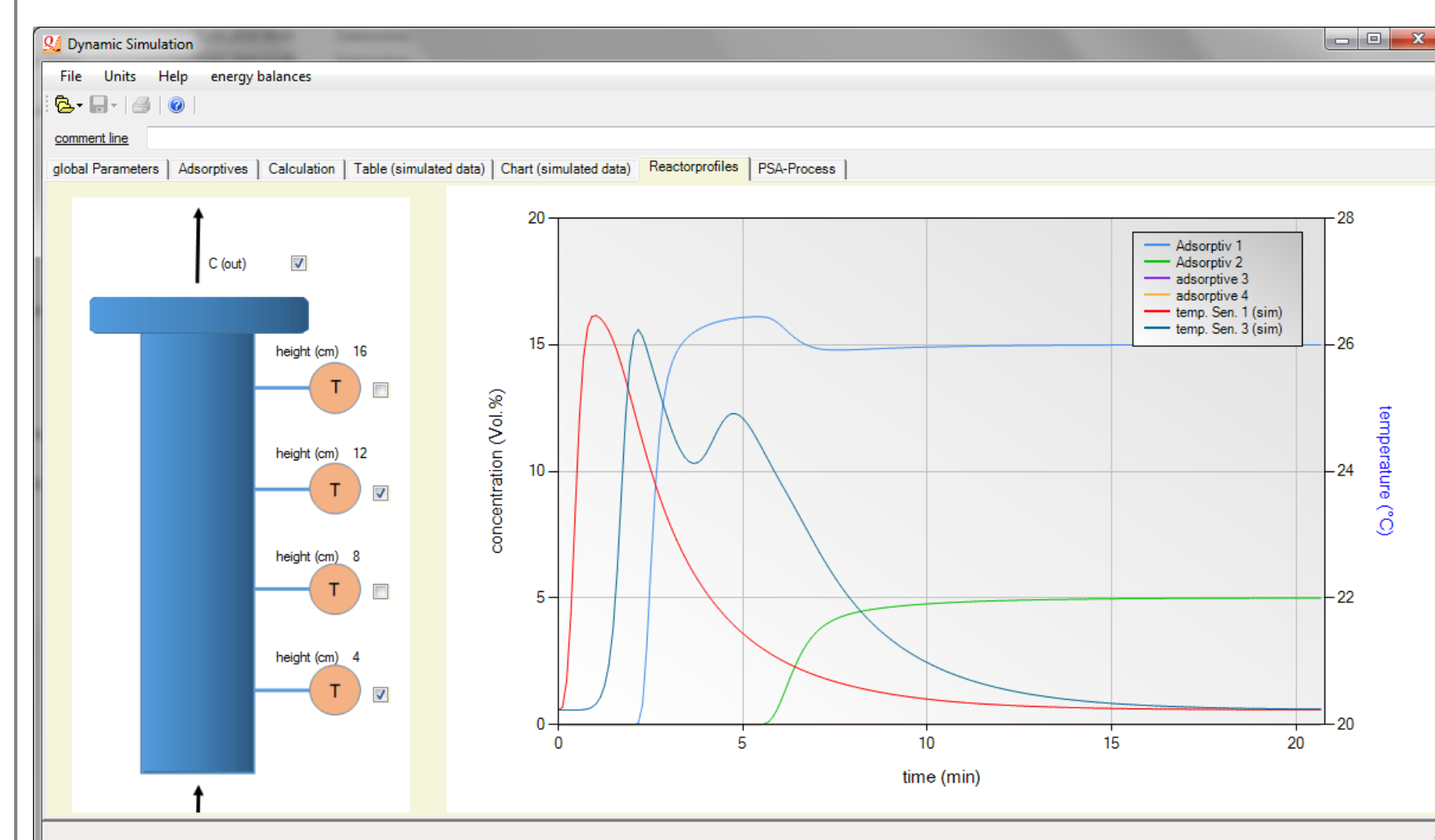
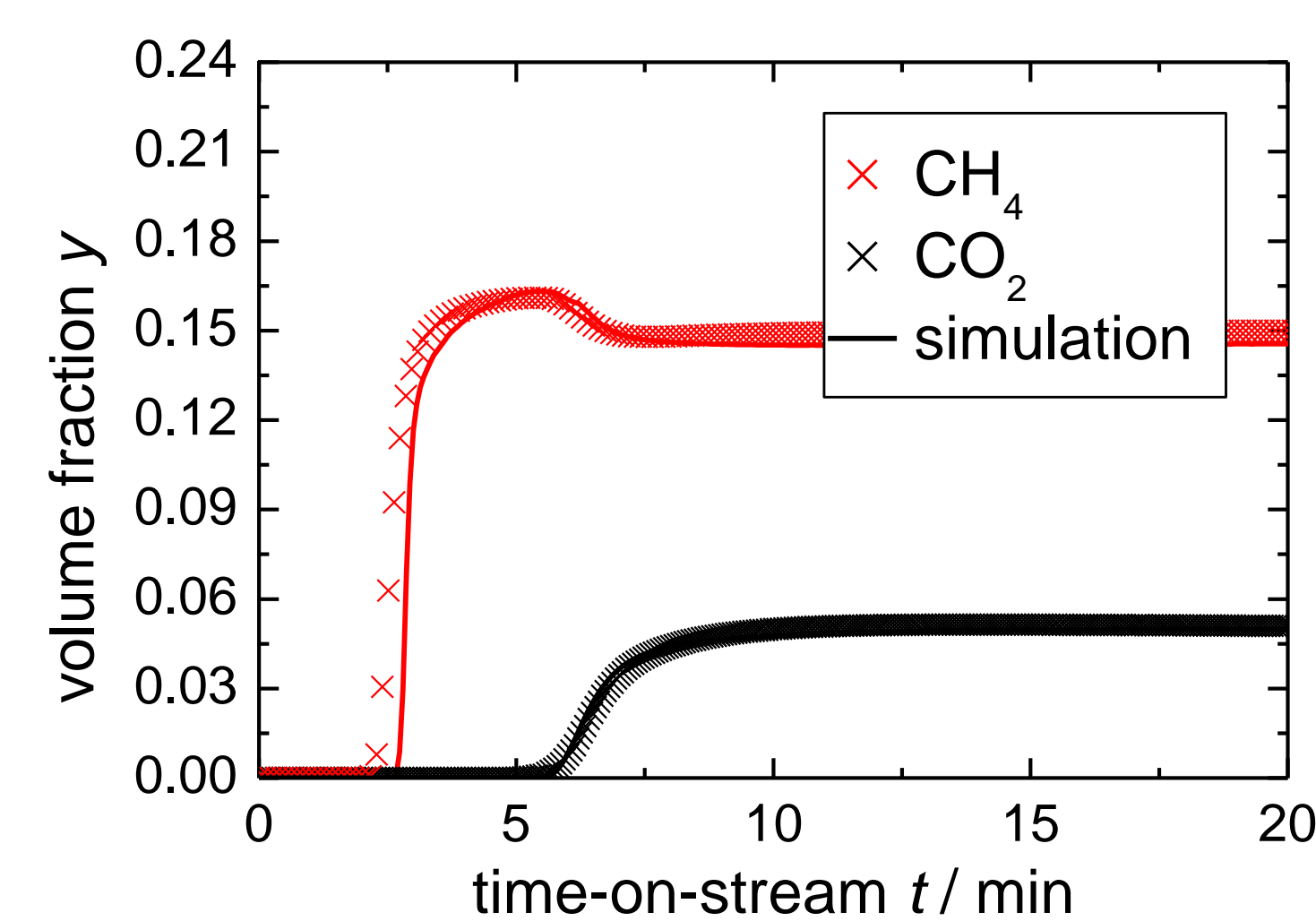


→ Mixture equilibria can be implemented in **Dynamic Simulations**.

*Ideal Adsorbed Solution Theory

Dynamic Simulation

- **dynaSim** provides a solver for mass- and energy balances which allows 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 dataset for **parametric studies**

*Linear Driving Force

Conclusions

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 technical 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.