

Multi-component adsorption of light hydrocarbons on different adsorbents at low temperature

Mats Roehnert¹, Sonja Schmittmann^{1,2}, Christoph Pasel¹, Christian Bläker¹, Dieter Bathen^{1,3}

¹University of Duisburg-Essen, Chair of Thermal Process Engineering, Lotharstr. 1, 47057 Duisburg, Germany

²Carbon Service & Consulting GmbH & Co. KG, Im Hasenfeld 12, 52391 Vettweiß, Germany

³Institute of Energy and Environmental Technology e. V. (IUTA), Bliersheimer Str. 60, 47229 Duisburg, Germany

Motivation

The removal of light hydrocarbons (C₂-C₄) at trace concentrations from exhaust air or process gas is important in various environmental and technical applications, e.g. processing of natural gas or separation of olefin/paraffin mixtures. Adsorptive processes are generally suitable for this purpose. Since adsorption is temperature-dependent, the thermodynamics and kinetics of the process can be optimized by varying temperature. As yet, no systematic

data are available on the multi-component adsorption of light hydrocarbons at low temperatures. Against this background, this work investigates the adsorption thermodynamics of light hydrocarbons on zeolites over a wide temperature range. In addition, multi-component adsorption is predicted by *Ideal Adsorbed Solution Theory* (IAST) using pure component data.

Materials & Methods

Experimental setup:

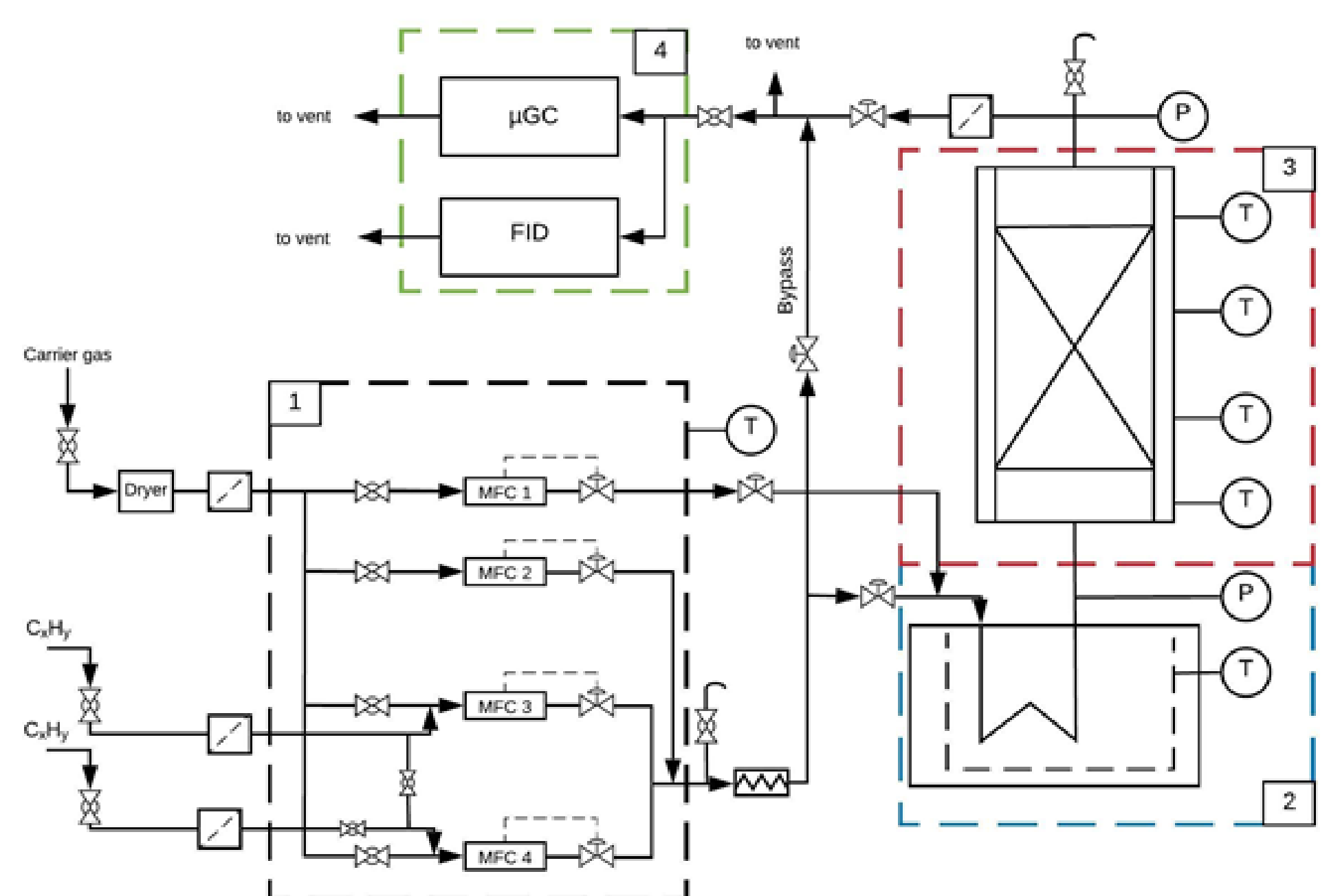
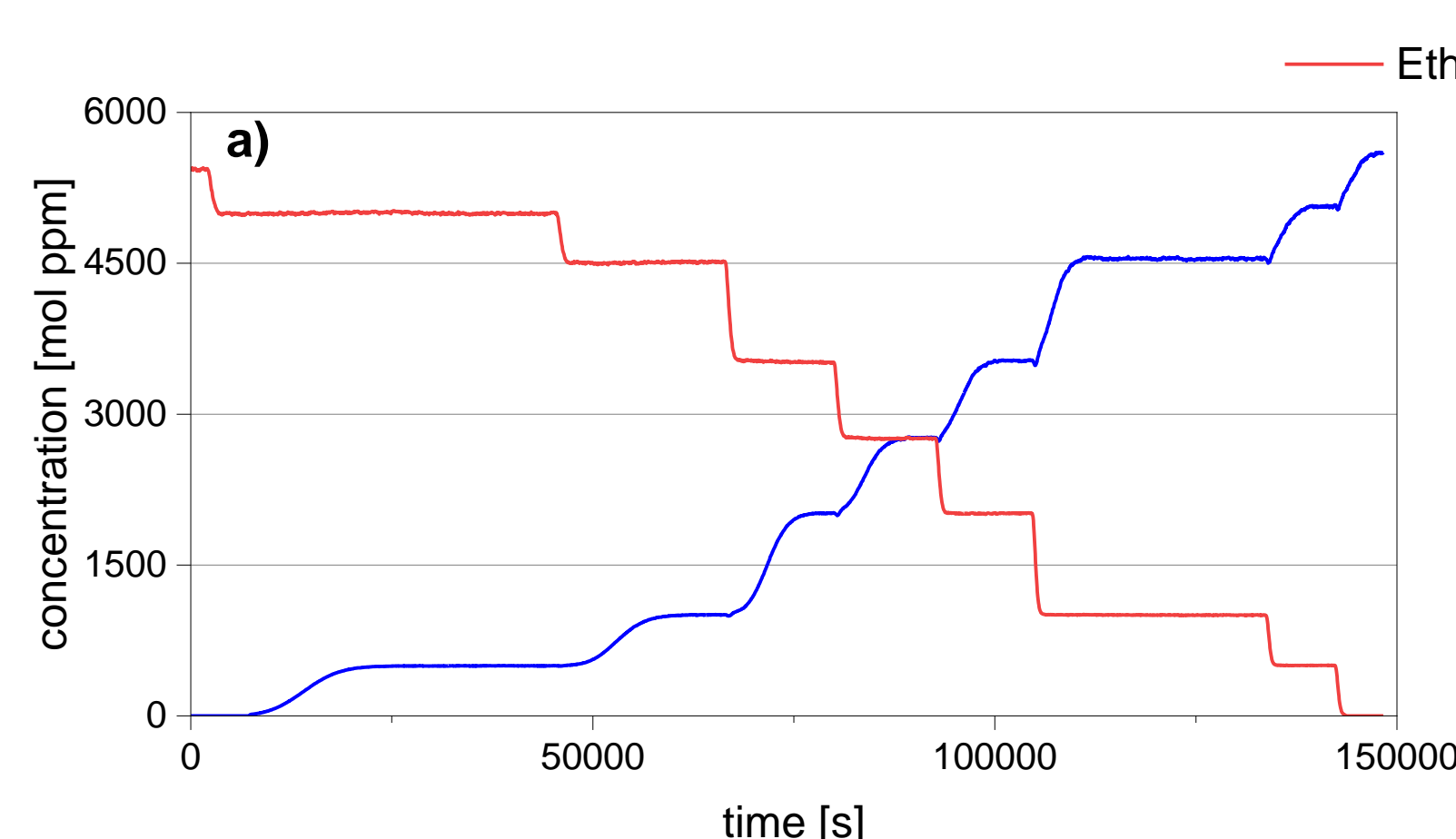


Fig. 1: Experimental setup

- C₂H₆/C₂H₄/N₂ mixture with mass flow controllers
- Cooling with cryogenic thermostat down to -80 °C
- Continuous gas analysis with gas chromatograph (μGC)

Methods:

Measurement of cumulative breakthrough curves



Calculation of adsorbent loading via mass balancing

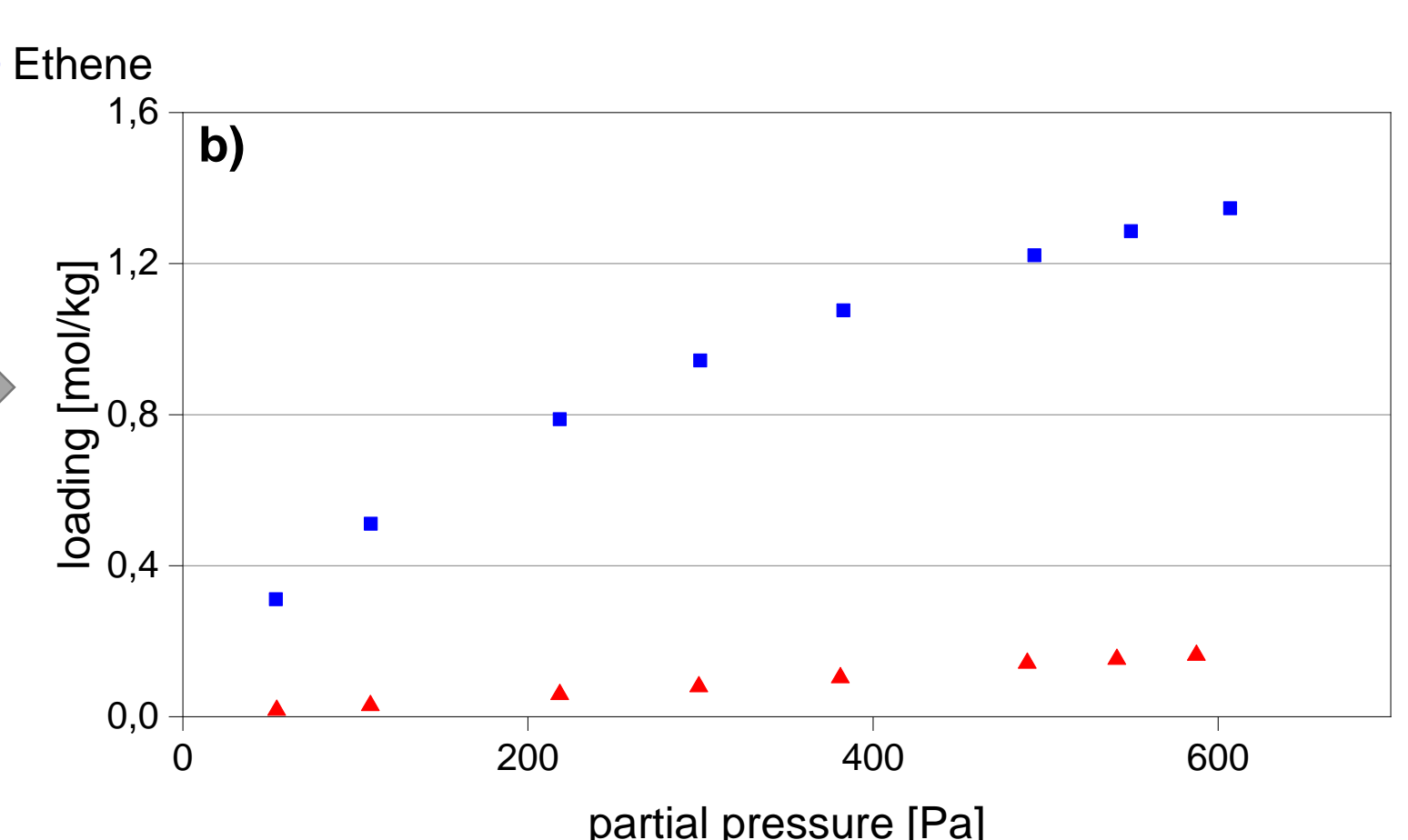


Fig. 2: Evaluation of a measurement a) adsorptive concentrations over time b) derived isotherms

- Isotherm description with temperature dependent Toth-isotherm:
$$X_{eq,i}(T, p_i) = X_{mon,i}(T) \cdot \frac{b_i(T) \cdot p_i}{(1 + (b_i(T) \cdot p_i)^{n_i(T)})^{1/n_i(T)}}$$

- Prediction of binary adsorption by *Ideal Adsorbed Solution Theory* (IAST) using pure component data

$$\frac{A \cdot \pi}{R \cdot T} = \int_0^{p_{i,0}} \frac{X_{eq,i}}{p_i} dp_i$$

Materials:

Adsorptives	Ethane - C ₂ H ₆	Ethene - C ₂ H ₄
Molar mass [g·mol ⁻¹]	30,07	28,05
Critical molecular diameter [Å]	4,48	3,40
Polarizability [c·m ² ·V ⁻¹]	4,47	4,25
Dipole moment [10 ⁻³⁰ C·m]	0	0
Quadrupole moment [10 ⁻⁴⁰ C·m ²]	0	6,67

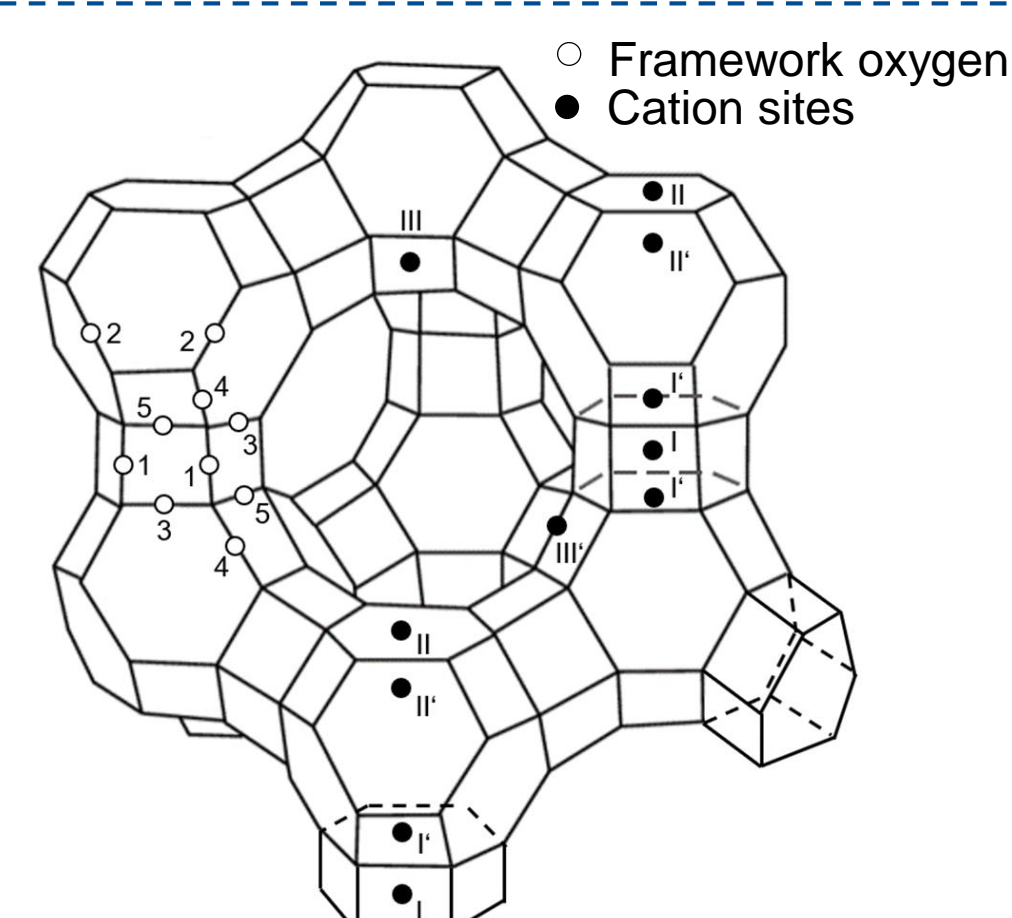


Fig. 3: Structure of a faujasite zeolite

Adsorbent: faujasite NaX

- Spherical pellets
- BET ~ 600 m²·g⁻¹
- Polar surface caused by exchangeable cations
- Homogeneous crystalline structure

Results & Discussion

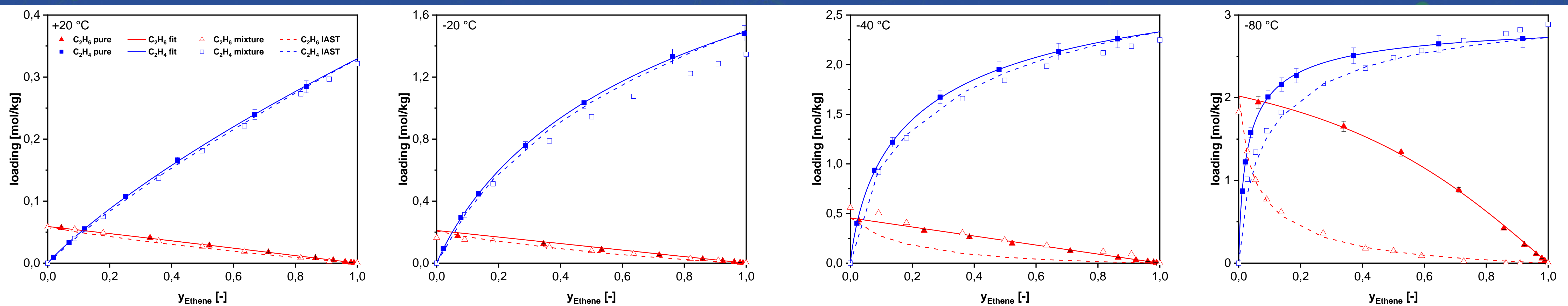


Fig. 4: Adsorption isotherms of ethane and ethene as pure components and in mixture at temperatures between +20 °C and -80 °C at a total partial pressure of 600 Pa

Binary adsorption:

- From +20 °C to -40 °C, the mixture isotherms almost reach the loading of the pure component isotherms. → No competition for adsorption sites
- At -80 °C, the ethane loading in the mixture decreases sharply at low mole fractions of ethene. → Ethene displaces ethane due to strong quadrupole-cation interactions
- Ethene reaches saturation at -80 °C, which leads to strong competition for adsorption sites. → Displacement depends on surface coverage

IAST prediction:

- Prediction of binary adsorption works well for the highest and lowest temperature.
- Very good prediction is obtained at -80 °C, though the isotherms of the pure components and the mixture isotherms differ strongly.

Summary & Prospect

To determine the effect of temperature on the binary adsorption of ethane and ethene at trace concentrations, isotherms were measured on NaX zeolite at temperatures between +20 °C and -80 °C. Over the entire temperature range, ethene reaches higher loadings than ethane, even at low fractions in the mixture. Between +20 °C and -40 °C, no displacement takes place because the loadings are very low and there are still sufficient adsorption sites available.

At -80 °C, the displacement of ethane by the stronger adsorbing ethene is pronounced, since the two hydrocarbons compete for the same adsorption sites. The IAST prediction of the binary adsorption is good.

Further work will investigate the influence of the zeolite structure and the exchange of cations on multi-component adsorption of hydrocarbons (C₂-C₄).