

Competitive high-pressure adsorption of CO₂/CH₄ mixtures on NIST reference zeolite Y (RM8850)

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The suitability of adsorbents for gas separation or storage depends mostly on adsorption equilibria and kinetics. For initial materials' screening, volumetric adsorption measurements at atmospheric pressures might be sufficient but for high-pressure applications, data at elevated pressures are essential. However, as shown in various studies in the literature (see, e.g., [1]), reproducibility of high-pressure adsorption investigations is challenging and often lacking, which relates to a lack of standardisation protocols, reference materials, and reference data. To address this issue, NIST initiated interlaboratory studies on high-pressure adsorption data of different unary gases on reference materials (see, e.g., CH₄ adsorption on reference zeolite Y (RM8850) [2]). Although this represents an important step forward, competitive adsorption of gas mixtures is more critical for industrial adsorption applications. Because of the inherent complexity of measurements with gas mixtures, their reproducibility still represents a major challenge in adsorption sciences.

This study aims to address this data gap by generating a set of competitive adsorption measurements with binary CH₄/CO₂ mixtures on the NIST reference zeolite Y (RM8850). We investigated unary adsorption isotherms for CO₂ and CH₄ at pressures up to 3 MPa and temperatures from (298 to 393) K using a magnetic suspension balance. We also measured the co-adsorption of binary gas mixtures with nominal initial CO₂ compositions of 25 mol%, 50 mol%, and 75 mol% over a similar pressure and temperature range. For data reconciliation, we applied co-adsorption models to estimate the competitive adsorption behaviour to yield a set of isotherm parameters and their uncertainty. In this endeavour, we also considered models that predict binary data based on the unary adsorption data. The rich experimental data set and the isotherm model parameters represent a useful point of departure for a database of co-adsorption on NIST reference materials.

[1] Broom DP, Hirscher M. Energy Environ Sci 2016;9(11):3368-80.

[2] Nguyen HGT, et al. Adsorption 2020;26(8):1253-66.