

Supporting Information for: Prediction of adsorption isotherms from breakthrough curves

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In this supporting information, we explain the empirical correlations used to estimate the effective mass transfer coefficient (k_L) and the axial dispersion coefficient.

1. Effective mass transfer and axial dispersion coefficients

The meaning of the effective mass transfer coefficient (k_L) depends on the highest resistance to mass transfer in a system. Silva et al. posed an effective LDF mass transfer coefficient including both external mass transfer as well as macropore diffusion [1]:

$$\frac{1}{k_L} = \frac{r_p}{3k_f} + \frac{r_p^2}{15D_{\text{eff}}} \quad (1)$$

Here r_p is the characteristic length of adsorbent particles (e.g. mean radius of particles for spherical particles), k_f is the film mass transfer coefficient, and the effective diffusivity D_{eff} is expressed as:

$$D_{\text{eff}} = \frac{\varepsilon_p}{\tau_f} D_p \quad (2)$$

where ε_p and τ_f are the porosity of the adsorbent and the tortuosity. The diffusion coefficient (D_p) can be written as a combination of Knudsen (D_K) and molecular diffusivity (D_M) [2, 3, 4]:

$$\frac{1}{D_p} = \frac{1}{D_K} + \frac{1}{D_M} \quad (3)$$

Further, D_K in turn can be written as [5]:

$$D_K = \frac{d_p}{3} \sqrt{\frac{8RT}{\pi M}} \quad (4)$$

where d_p is the nominal pore diameter of adsorbent, M is the molar mass of adsorbate, R is the universal gas constant and T is the temperature. For the estimation of molecular diffusion coefficients, one could e.g. use the group-contribution methods provided by Poling et al. [6]. The value 15, (right-hand side of Eq. 1) was first derived by Glueckauf [7], by comparing theoretical chromatograms of different mass transfer models. The same value (15) has been recommended for process design by Ruthven [8]. Although this value is not appropriate for very short cycle times [9], it is sufficient for breakthrough simulations in this work.

The axial dispersion coefficient can be estimated knowing the Schmidt and Reynolds numbers [10, 11]. Axial dispersion is caused by two spreading mechanisms: (1) molecular diffusion (2) eddy diffusion. In general, the axial dispersion coefficient is a function of Reynolds number and therefore it changes along the column when appreciable amounts are adsorbed. At low Reynolds number, the molecular diffusion is the main spreading mechanism in the axial direction and the effect of eddy diffusion can be neglected [12, 13]. The molecular diffusion coefficient is given by [14]:

$$D_{M,g} = \frac{CT^{1.5} \sqrt{\frac{1}{M_1} + \frac{1}{M_2}}}{p\sigma_{12}^2\Omega} \quad (5)$$

where C is a constant, M_i is the molar mass of component i , $\sigma_{ij} = (\sigma_i + \sigma_j)/2$ is the average collision diameter and Ω is the temperature-dependent collision integral.

2. Adsorption isotherm Henry region

The experimentally measured adsorption isotherm of pure CO_2 and CH_4 at 298 K in zeolite ITQ-29 are shown in Fig. 1.

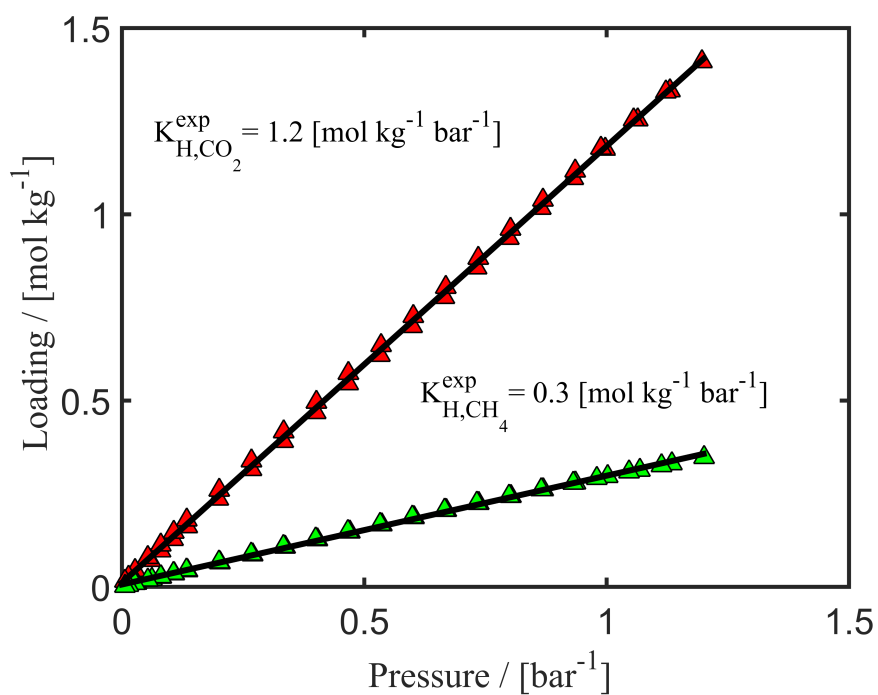


Figure 1: Experimentally measured adsorption isotherm of pure CO_2 and CH_4 at 298 K in zeolite ITQ-29. Symbols show the experimentally measured values. The Henry coefficients are obtained by the slope of the line fitted to the data points (solid lines).

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