

Auxiliary Material: Determination of total amount of adsorbed fluid

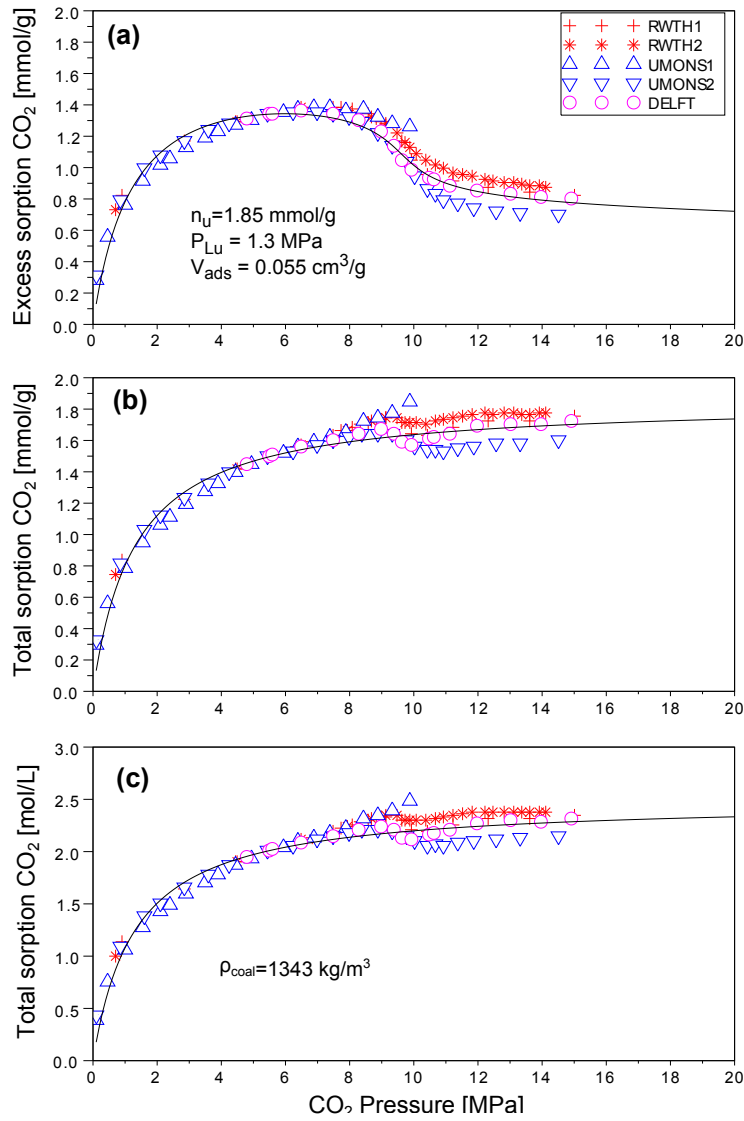
We follow the procedure described by Ottiger et al. [2006]. Total sorption n_T [mol/g] can be approximated as the summation of excess sorption n_{ex} [mol/g] and the fluid mass not-in-excess in the volume of the adsorbed phase, proportional to the volume of the adsorbed phase per unit mass of coal V_{ads}/m_{coal} [cm³/g] and the bulk mass density of the fluid ρ_b [mol/cm³]:

$$n_T = n_{ex} + \frac{V_{ads}}{m_{coal}} \rho_b$$

If n_T is assumed to follow a Langmuir trend (reasonable for low-medium pressure), then, n_{ex} can be fitted with three parameters n_u , P_{Lu} , and V_{ads}/m_{coal} :

$$n_{ex} = n_u \frac{p}{p + P_{Lu}} - \frac{V_{ads}}{m_{coal}} \rho_b$$

The following figure shows the three parameter fitting of the experimental data presented by *Gensterblum et al.* [2010] for Brzeszcze coal. The fitting permits recovering an estimate of the adsorbed phase volume per unit mass of coal $V_{ads}/m_{coal} = 0.055$ cm³/g, which can be used to estimate the total sorption amount n_T .



Determination of total adsorption amount for coal immersed in the adsorbate (unjacketed) at 45°C. (a) Excess sorption [mmol/g] measured for Brzeszcze coal by different laboratories (symbols - *Gensterblum et al.* [2010]) and 3-parameter Langmuir fitted model. (b) Total sorption amount adding the mass of fluid (V_{ads}/m_{coal}) ρ_b (CO_2 bulk mass density computed from EOS *Span and Wagner* [1996]). (c) Total adsorption amount per unit volume of undeformed specimen [mol/L] obtained with $\rho_{coal} = 1343$ kg/m³.