Modelling water adsorption isotherms obtained from smectite interlayer nanopores

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Clay and clayey materials are commonly analysed with XRD to determine the basal spacing, state of hydration and intercalation processes. Through the investigation of these parameters combined with the dependency on the interlayer solutes and ions, a deeper knowledge of the long- and short-term effects of water exposure can be attained. In instances where XRD measurements are not applicable or the desired information cannot be attained alternative methods are necessary.

In this study a theoretical and step-wise model is constructed to predict the water uptake of the smectite clay mineral montmorillonite based on gravimetric adsorption isotherms in a range of 0-98% RH. Eight samples of homo-ionic, purified MX-80 bentonite was prepared with both mono- and divalent cations (Li, Na, K, Cs, Mg, Ca, Cu, Sr).

The calculations are made using two water adsorption equations, the Dubinin-Astakhov[1] and Do & Do's[2] adsorption model. The former calculates intercalated water whereas the latter accounts for the remaining adsorbed water.

Based on how the mass-uptake depends on the humidity for the individual samples it was found possible to model how the corresponding adsorbed water is distributed in integers of overlapping water monolayers (0,1,2,3). This results in a unique ion dependent profile that can be compared and confirmed with traditional XRD measurements versus %RH, which can then be used to extract useful information of the systems as a whole or as unique homo-ionic samples.

The theoretical basal spacings obtained from the model was found well in line with traditional XRD measurements. Furthermore, the data from the homo-ionic samples demonstrated a trend of increased water uptake and monolayer formation with decreasing size for alkali metals, whereas the monolayer formation occurs at lower %RH with increasing size for alkali earth metals.

References:

1. Do, Duong D. Adsorption Analysis: Equilibria and Kinetics. Imperial College Press: London, 2008.
2. Do, D. D., Junpirom, S. & Do, H. D. A new adsorption-desorption model for water adsorption in activated carbon. *Carbon N. Y.* **47,** 1466–1473 (2009).