Errata 2011-10

SKB R-10-48

Bedrock K_d data and uncertainty assessment for application in SR-Site geosphere transport calculations

In the earlier distributed report, there are errors that have now been corrected. The corrected page 32 is enclosed. The changed text is marked with a vertical line in the page margin. An updated pdf version of the report, dated 2011-10, can be found at www.skb.se/publications.

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plexation reaction at equilibrium. It should be noted that although the intrinsic constant K_{int} does not change with solution ionic strength, the apparent equilibrium constant, K_{app} is influenced by ionic strength (and therefore only a *conditional constant*). When deriving protonation/deprotonation and solute binding constants for a variably charged surface it is therefore important to be able to separate the chemical and Coulombic contributions.

In general, all SCM's use the same electrostatic correction factor as defined by Equation 2-31. The main difference between the various SCM's, however, depends mainly upon how the spatial distribution of covalently bonded and electrostatically bonded counter ions is conceptualised. The implicit assumptions in these have consequences for how electrical potential is calculated and the range of phenomena that can be modelled. The different main types of surface complexation models that are discussed in the literature fall into the types illustrated in Figure 2-6.

The simplest model that can be conceptualised, however, neglects electrostatic charge entirely and simply models the surface complexation reactions using conditional equilibrium constants that are not corrected for electrostatic effects. This is referred to as a non-electrostatic model (NEM). Since the thickness of the electrical double layer and consequently, the work required moving charges from the bulk solution to the interface is dependent on ionic strength, one implication of the NEM is that ionic strength effects cannot be modelled and the model is only strictly valid for an approximately fixed groundwater ionic strength.

Constant Capacitance Model (CCM)

In the constant capacitance model (CCM) /Schindler et al. 1976/, it is assumed that both specifically adsorbed ions as well as electrostatically bound counter ions are held tightly in a single layer at a distance exactly adjacent to the surface and no distinction is made between the o- and β-planes and the diffuse layer. The surface potential, ψ_0 is calculated by assuming that it is balanced by a layer of counter-ions in a physical analogue to a parallel plate capacitor. In this physical model, the variation of electrical potential with distance is linearly related to the surface charge by way of the capacitance of this layer which is treated as a fitting parameter:

$$\sigma_p\ (\mathrm{C/m^2}) = C\psi_0 \qquad (2\text{-}32)$$

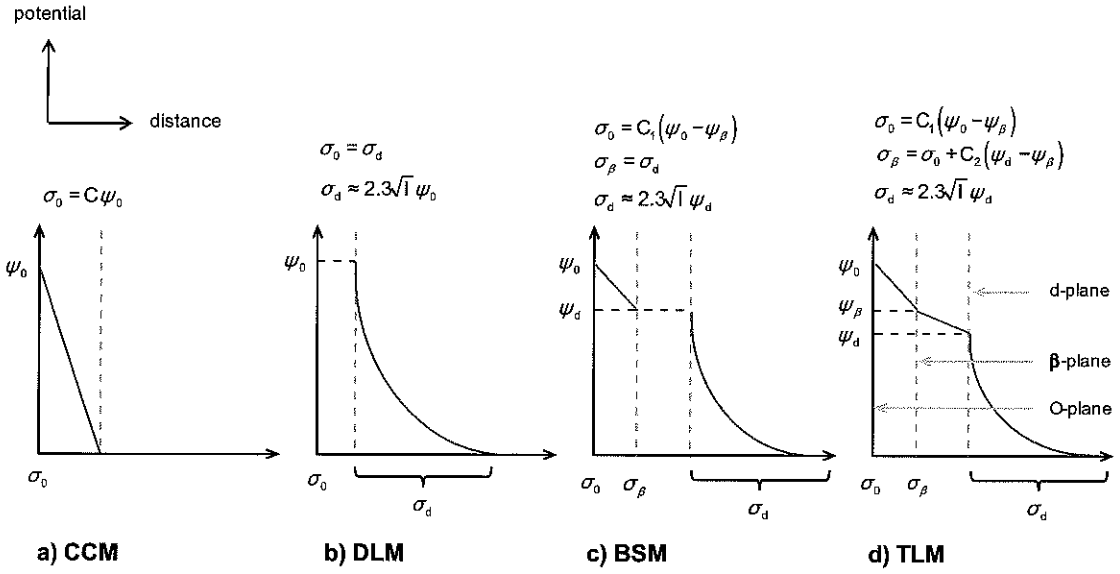

Figure 2-6. *Illustration of different types of surface complexation models differing mainly in the conceptualisation of surface charge. Models shown are a) constant capacitance model (CCM), b) double layer model (DLM), c) basic Stern model (BSM), and d) triple layer model (TLM).*