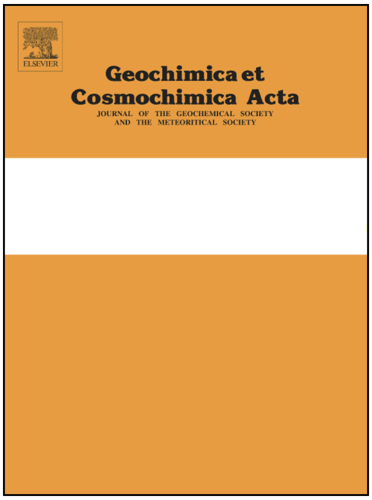

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A general framework for ion equilibrium calculations in compacted bentonite

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Abstract

An approach for treating chemical equilibrium between compacted bentonite and aqueous solutions is presented. The treatment is based on conceptualizing bentonite as a homogeneous mixture of water and montmorillonite, and assumes Gibbs-Donnan membrane equilibrium across interfaces to external solutions. An equation for calculating the electrostatic potential difference between bentonite and external solution (Donnan potential) is derived and solved analytically for some simple systems. The solutions are furthermore analyzed in order to illuminate the general mechanisms of ion equilibrium and their relation to measurable quantities. A method is suggested for estimating interlayer activity coefficients based on the notion of an interlayer ionic strength. Using this method, several applications of the framework are presented, giving a set of quantitative predictions which may be relatively simply tested experimentally, e.g.: (1) The relative amount of anions entering the bentonite depends approximately on the square-root of the external concentration for a 1:2 salt (e.g. $CaCl_2$). For a 1:1 salt (e.g. NaCl) the dependence is approximately linear, and for a 1:2 salt (e.g. Na_2SO_4) the dependence is approximately quadratic. (2) Bentonite contains substantially more nitrate as compared to chloride if equilibrated with the two salt solutions at equal external concentration. (3) Potassium bentonite generally contains more anions as compared to sodium bentonite if equilibrated at the

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