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A general framework for ion equilibrium calculations in compacted bentonite

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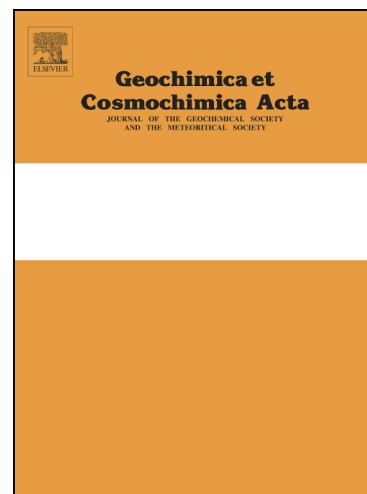
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# 1 A general framework for ion equilibrium calculations in 2 compacted bentonite

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## 5 Abstract

6 An approach for treating chemical equilibrium between compacted bentonite  
7 and aqueous solutions is presented. The treatment is based on conceptualiz-  
8 ing bentonite as a homogeneous mixture of water and montmorillonite, and  
9 assumes Gibbs-Donnan membrane equilibrium across interfaces to external  
10 solutions. An equation for calculating the electrostatic potential difference  
11 between bentonite and external solution (Donnan potential) is derived and  
12 solved analytically for some simple systems. The solutions are furthermore  
13 analyzed in order to illuminate the general mechanisms of ion equilibrium  
14 and their relation to measurable quantities. A method is suggested for es-  
15 timating interlayer activity coefficients based on the notion of an interlayer  
16 ionic strength. Using this method, several applications of the framework are  
17 presented, giving a set of quantitative predictions which may be relatively  
18 simply tested experimentally, e.g.: (1) The relative amount of anions enter-  
19 ing the bentonite depends approximately on the square-root of the external  
20 concentration for a 1:2 salt (e.g.  $\text{CaCl}_2$ ). For a 1:1 salt (e.g.  $\text{NaCl}$ ) the  
21 dependence is approximately linear, and for a 1:2 salt (e.g.  $\text{Na}_2\text{SO}_4$ ) the  
22 dependence is approximately quadratic. (2) Bentonite contains substantially  
23 more nitrate as compared to chloride if equilibrated with the two salt so-  
24 lutions at equal external concentration. (3) Potassium bentonite generally  
25 contains more anions as compared to sodium bentonite if equilibrated at the

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