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Influence of Cations on the Dissolution of Apatite: a Combined Experimental and Computational Approach

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Apatite is a mineral present in various geochemical environments (soils, sediments, etc.,), in part of biogenic origin (bone, etc.). The property of apatite to trap the hazardous metals is widely used in medicine, polluted sites decontamination and nuclear waste management. The stability of apatite is an important parameter, which depends on the environmental conditions (Misra et al, 1975). In laboratory experiments, the effect of foreign cations on the dissolution rate of synthetic hydroxyapatite was measured in flow-through reactor. This technique is well suited for investigation of reaction kinetics as a function of solution composition (Van Cappellen et al., 1997), as it allows to study simultaneously the sorption of the cation at trace level concentration and the dissolution rate. In contrast to batch reactor, the method eliminates the interference of possible back reactions due to the accumulation of reaction products. Experimental results are shown in the Fig. 1. An increased concentration of Zn^{2+} in the reactor results in a decreased apatite steady state dissolution rate. Similar experiments performed with other cations indicate: - a decrease of dissolution rate with an increase of metal surface coverage of apatite particles - a distinct effect among cations depending on their size and electronic properties. Molecular dynamics were used to characterise this effect, and in particular to model the sorption reaction mechanism initial step. The co-ordination sphere of the cation changes as the ion approaches the hydroxyapatite surface, even before the formation of a chemical bond to the surface. As the ion, initially hexa-coordinated with water molecules, approaches the apatite channel, an inner-sphere surface complex is formed. This reaction is expected to lead to the sorption *per se*, i.e., to the replacement of Ca^{2+} ions on the surface or along the apatite "channels" by foreign metal cation. As a consequence of this inhibitions mechanism, the dissolution of archaeological bones will be shown, in another communication to be related to the presence in these bones (Reiche et al, 1999) of various trace metal cations ($Fe^{2+/3+}$, Mn^{2+}, Sr^{2+}). Various mechanisms such as adsorption, diffusion or surface precipitation may be involved.

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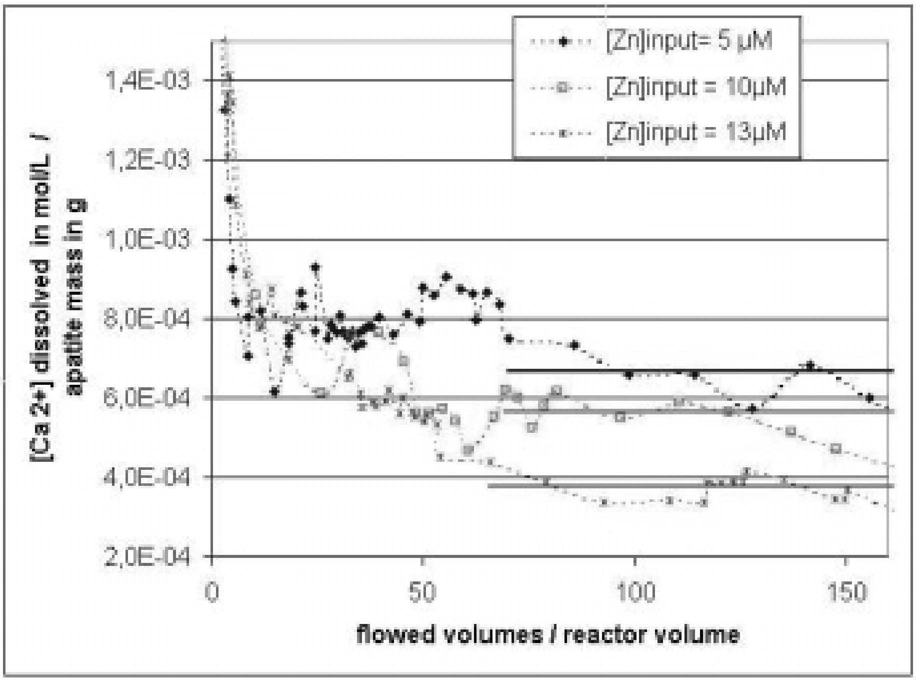

Figure 1:Effect of Zn concentration on the apatite dissolution at 25 C, pH = 5.3 and I = 0.01 mol/L