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Interaction of Fe(II) with cement phases in anoxic conditions

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Thermodynamic modeling is a powerful tool capable of predicting the mineralogical and chemical composition of cementitious systems [1]. At present, however, these properties cannot be adequately modelled under anoxic conditions due to the lack of thermodynamic data for reduced Fe species interacting with cement phases. Reduced iron plays an important role in low and intermediate-level waste (L/ILW) repositories as redox conditions will be reducing in the long term due to the presence of large amounts of steel. Fe(II) released from corroding steel reinforcement and canisters, into the cement matrix could be either taken up by cement phases in a manner similar to Fe(III), which substitutes for Al(III) in cement phases [2,3], precipitate as specific Fe(II)-bearing phase, e.g. Fe(II)-hydroxide or Fe(II)-sulfides, or adsorb onto the surface of cement phases.

Sorption experiments with Fe(II) and Fe(III) were carried out on the most important cement phases using ^{55}Fe as radiotracer. In addition, Fe(II)-bearing C-S-H, AFm and AFt phases were synthesized and characterized to account for complete (end-member) and partial replacement (solid solution) of Ca^{2+} by Fe^{2+}. EXAFS spectroscopy was employed to determine the coordination environment of Fe(II) in the sorption samples and the Fe(II)-doped cement phases.

In this work, we present the experimental results and discuss their relevance in the context of thermodynamic modelling of cementitious materials for application in safety assessment of cement-based repositories for radioactive waste.

[1] Lothenbach & Winnefeld (2006) *Cem. Concr. Res.* **36**, 209-226. [2] Dilnesa *et al.* (2014) *Cem. Concr. Res*. **58**, 45-55. [3] Vespa *et al.* (2015) *J. Am. Ceram. Soc*. **98**, 2286-2294.