INCORPORATION OF HEAVY METALS (Co, Cu, Zn) IN SYNTHETIC CALCIUM-ALUMINIUM-SILICATE-HYDRATE (C-A-S-H) GEL STRUCTURES: ENVIRONMENTAL IMPLICATIONS FOR METAL ION TRANSPORT IN AQUEOUS MEDIA

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Concrete is one of the most important building materials of our time. During cement hydration, exposure of cementitious materials to heavy metal (Me) ions can cause severe environmental risks, taking that novel cement supplements (slag, fly ash, etc.) can carry much higher levels of potentially hazardous Me ions than ordinary Portland cement (ACHTERNBOSCH et al., 2003). The focus of our study is to investigate the immobilization mechanisms and thresholds of Me ions during the co-precipitation with calcium-aluminium-silicate-hydrate (C-A-S-H) gels, as well as revealing apparent changes in the physicochemical properties of such Me-doped phases. Therefore, C-A-S-H bearing Me ions were synthesized from Si-, Ca-, Al- and Me-salts by a sol-gel process with given molar ratios of Ca/Si (1.0) and Al/Si (0.05), but varying molar ratios of Me/Si (0 to 0.6). During C-A-S-H phase precipitation and maturation, monitoring of the reactive fluid chemical composition was performed by pH and ICP-OES analyses. The crystal chemistry-structure relationships of the precipitates were characterized by FTIR, XRD, ESEM, TEM and thermogravimetric analyses. The formation of poorly crystallized, nano-sized (40 to 60 nm) C-A-S-H particles with a homogeneous chemical (gel-like) composition in the range from 0.87 to 0.99 of molar (Ca+Me)/(Si+Al) was observed at Me ion concentrations lower than 0.4 M. At higher Me ion loads of copper (Cu^{2+}) (> 0.4 M) the co-precipitation of reaction by-products, such as atacamite ($Cu_2Cl(OH)_3$), has been observed, which denotes the upper level of Me ion immobilization by synthetic C-A-S-H gel structures. The removal mechanism is based on isomorphous substitution of the respective Me ion for the Ca position in the CaO layer of the C-A-S-H structure (1 to 40 mol% substitution of Me for Ca), though a minor amount of interlayer ion exchange is possible (BALDERMANN et al., 2019). This indicates that Me ions preferentially substitute for Ca in the C-A-S-H structure, thus reducing the risk of contamination of the environment. Further efforts will focus on calculating respective solubility products in order to shed light on the physicochemical properties and chemical reactivity of C-A-S-H bearing low to extremely high loads of heavy metals.

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