Goldschmidt 2021 Abstract
https://doi.org/10.7185/gold2021.5837

Investigating the hydration of tricalcium aluminate in the presence of chromate and selenate anions

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Ettringite ($Ca_6[Al(OH)_6]_2(SO_4)_3.26H_2O$) and calcium aluminate monosulfate ($3CaO{\cdot}Al_2O_3{\cdot}CaSO_4{\cdot}12H_2O$) are hydration products of ordinary portland cement (OPC). They have well characterised crystal structures. Ettringite's structure consists of cation columns with composition $(Ca_3[Al(OH)_6].12H_2O)^{3+}$, that run parallel to the *c* axis, with the sulfate anions and remaining water molecules in channels parallel to these columns [1]. Calcium aluminate monosulfate has a hexagonal crystal structure made up of layers of $(Ca_3[Al(OH)_6]_2)^{2-}$ with sulfate and water in the interlayer [2].

Both ettringite and calcium aluminate monosulfate have known analogue phases [3]. This study has synthesised analogue phases of the ettringite structure with chromate (CrO_4^{2-}) or selenate (SeO_4^{2-}) in place of the sulfate (SO_4^{2-}) anions in the channels, and an analogue phase of calcium aluminate monosulfate with chromate in place of the sulfate anions between the layers. Precipitation of these analogue phases could be used to remediate water polluted with hexavalent chromium or selenium, which are hazardous to human health and the environment.

In OPC, tricalcium aluminate (C3A, $Ca_3Al_2O_6$) hydrates in the presence of gypsum ($CaSO_4.2H_2O$), forming ettringite. After the sulfate has been consumed, the formed ettringite will react with more C3A to form calcium aluminate monosulfate [4]. This study uses the hydration of C3A in solutions containing either chromate or selenate anions to form ettringite and calcium aluminate monosulfate analogue phases.

The reaction pathway was fully investigated by altering the concentration of the solutions and the reaction time. Solid samples, taken at various reaction times, were characterised using PXRD, FTIR and ICP-OES to determine what phases had formed. The method was found to remove the chromium and selenium from the solutions and ettringite and calcium aluminate monosulfate analogue phases were identified in the solid products. A pure sample of calcium aluminate monochromate ($3CaO{\cdot}Al_2O_3{\cdot}CaCrO_4{\cdot}14H_2O$) was synthesised and using high resolution powder X-ray diffraction data, a structural model has been proposed.

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