

ESTIMATES OF MISSING MINERAL STABILITY CONSTANTS FOR LESS COMMON ELEMENTS FROM pH DEPENDENCE LEACHING TEST DATA

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In geochemical modelling of soils, wastes, recycled materials and cementitious products, the appropriate stability constants for environmentally relevant elements are missing or insufficiently accurate, which makes modelling of long-term release of such elements difficult. Earlier, constants describing Ba, Sr and oxyanion (As, B, Cr, Mo, Sb, Se, W, V) substitution in ettringite have been derived using pH dependence test data (EN 14429 and EPA 1313) of a wide range of alkaline materials and experimental conditions. In the meantime, additional ettringite substitution parameters have been derived for Be, Cs, Tc and CN⁻. This approach of filling gaps in release behaviour of elements in pH dependence test data based on analogies in behaviour of elements, for which appropriate thermodynamic data are available is the basis of the current paper. Multi-element geochemical speciation modelling of pH dependence test data of materials and products of interest form the basis for deriving estimated values by an iterative approach once an adequate description of major and minor elements has been achieved. An example is arsenocrandalite, based on which similar phases for Sb, Se, V, Mo have been derived. Based on the existing mineral of the type Ca_x[OH]_y[AsO₄]_z corresponding phases for Cr, Mo, Sb, Se and V have been derived for the high pH domain for neutral to mildly alkaline materials where ettringite does not play a role. Phases of the type CaCO₃.XXCO₃ have been derived for Ba, Be, Li, Mg and Sr in a range of different highly carbonated materials and products. Friedel salt stability can be used as a starting point for other halogens, as well as for cyanide. The latter provided in combination with CN⁻-ettringite substitution a good description of alkaline CN⁻ contaminated soil. Thermodynamic stability constants for tungsten are scarce. Since tungsten has similar chemistry as molybdate, tungstate solubility can be described with corresponding molybdate phases, such as CaMoO₄ and PbMoO₄, for which stability constants are available. Filling gaps on the basis of reasonable assumptions for potential minerals can improve the understanding of release in reactive transport of less common elements until more specific thermodynamic data can be obtained.