Use of Chemical Speciation and Mass Transport Models in Leaching Assessment of Coal Combustion Residues in Agricultural Applications

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Abstract

With the development and use of standardized characterization leaching tests (LEAF) new possibilities for more detailed understanding of release controlling processes and insight in release controlling mineral and sorptive phases is possible through geochemical modelling. Since the release behaviour of individual substances is affected by major, minor and sometimes trace constituents in the material, insight in release controlling processes requires an integrated evaluation of a material as a whole. In case coal combustion residues (CCR) are added in a certain proportion to other materials to form a new blend with beneficial properties, the components in the mix and the blend need to be tested initially to be able to identify the factors that result in possible changes in the release behaviour of the blend. This then provides the possibility to vary mixing ratios to optimize environmental performance.

For geochemical speciation and chemical reaction/transport, the modelling framework LeachXS-ORCHESTRA (Objects Representing CHEmical Speciation and TRAnsport models) is used, which includes thermodynamic stability data for minerals and other solubility controlling parameters such as binding to Fe-oxide, Al-oxide, dissolved organic carbon and particulate organic matter. LeachXS has been developed to facilitate data retrieval, test comparison, geochemical modelling and scenario evaluation. For agricultural applications, modelling provides insights into mechanisms and extent of constituent liquid-solid partitioning and leaching under equilibrium and percolation conditions.

Based on pH dependence test data Chemical Speciation Fingerprints can be determined for any given material, which can subsequently be used for modelling of release from mixtures, reactive transport in percolation or diffusion scenarios and complex multilayer models.

The coupled characterization and geochemical speciation approach has been applied to cement based products containing varying proportions of coal fly ash, but also for coal fly ash use as an amendment for soil improvement. The traditional evaluation based on total content is not adequate to properly address release as there is often no correlation between total content and leachability because of partial incorporation of trace species into recalcitrant phases or largely irreversible sorption. Focussing only on the constituents of potential concerns is not useful either as release of such substances is largely controlled by the matrix chemistry of the resulting mixture (i.e., a combination of solution complexation, partially soluble solid phases and reversible sorption onto mineral surfaces or particulate organic matter).