

OP 1.6

Chemical speciation fingerprints by geochemical modelling after the characterisation of the leaching behaviour of various materials

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The characterisation of materials, such as soil, contaminated soil, sediments, sludge, compost, wood, waste and construction products, is entering a new phase with the latest developments in characterisation leaching tests and associated chemical speciation modelling capabilities. The increased insight in contaminant release controlling processes shows that the release of contaminants from materials largely depends on the chemical speciation of constituents. Therefore, geochemical reaction/transport modelling forms the basis for prediction of long term release behaviour and chemical partitioning of elements between different chemical binding forms (chemical speciation fingerprint). Using proper thermodynamic stability data and other solubility controlling parameters allows quantification of binding to Fe-oxide, Al-oxide, dissolved organic carbon and particulate organic matter and minerals. For geochemical speciation/ transport, the modelling framework ORCHESTRA (Objects Representing CHEmical Speciation and TRANsport models) (Meeussen, 2003) coupled to LeachXS as the data management system is used.

Proper waste management, satisfying environmental and health related criteria, requires a fair amount of information on a wide range of materials/substances. This information involves a proper material description, composition data, physical properties of a material, data on leaching of inorganic and organic constituents and, whenever relevant, biological properties. Release of constituents through leaching is a key aspect for judging environmental impact of material management options focussed on beneficial applications as well as on disposal, because most pathways of transport go in one way or another through a dissolution phase. The database/expert system (LeachXS) has been developed to facilitate data retrieval, test comparison, geochemical modelling and scenario evaluation using a full mechanistic description of processes.

The pH dependent leaching behaviour in combination with the calculated chemical speciation of constituents in the solid phase and in solution allows judgement of the bioavailability of constituents through their distribution between the free and DOC-bound fraction in solution. For judgement of treatment options, this means of assessing changes in material behaviour is potentially very powerful to make the right choices. For impact assessment this approach allows far better and more realistic predictions of environmental impact than the use of a constant factor that describes the distribution of contaminants between the liquid and solid phase ("K_d concept").