Perspective

Mineralogy and pollutant-trapping mechanisms

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Following in the footsteps of Ettler and Johan [7], Ettler et al. [8], whose work demonstrated the importance of having a sound knowledge of the mineral species derived from processing waste in the aim of optimising management, this note underlines the vital role that mineralogy plays in waste management. Mineralogy forms an integral part of the approach necessary for mineral waste definition, designing and certifying stabilization processes for pollutants, and long-term prediction. The strategy involved in its implementation comprises three main aspects: (a) *assessment*, with characterization of the bonds between the pollutant and the trapping chemical compound; (b) *anticipation*, with a search for the most likely structure to trap the pollutant under given physicochemical conditions; (c) *prediction*, with hypotheses that can be put forward concerning pollutant stability, through comparison with equivalent natural substances and using computing codes to simulate degradation for pre-established scenarios.

Assessment comprises the characterization of the bonds between the pollutant and the trapping chemical compound, as recently emphasized by Cases and his team [3,4,16]. A variety of tools are available that can give information from the macro-scale to the bonding scale: microscopy; X-ray diffraction (XRD); Electron Microprobe (EM) enabling in situ microanalysis (some μm^3); Scanning Electron Microscope (SEM),

and Transmission Electron Microscope (TEM), aimed at visualizing mineral shape and heterogeneity. Finally, at bonding scale with the availability of particle accelerators (X-photons, protons), we have the spectroscopy tools based on electromagnetic waves (*s.l.*): Mössbauer, EXAFS/XANES, Electronic Paramagnetic Resonance, Nuclear Magnetic Resonance, etc. [2]

Anticipation actions aimed at trapping potentially toxic substances can be classified into three types: (a) use of a known stable mineral structure to create an artificial structure with similar physicochemical characteristics; (b) use of knowledge concerning mineral solid-solution properties to create a structure able to trap pollutants; (c) use of Earth Science knowledge concerning the stability of mineral phases in the surficial environment (saturated and unsaturated zone), with the aim of optimising stabilization processes depending on the implementation constraints of the products.

Moreover, the interest of mineralogy lies in studying the relationships that exist between the structures and their physical and chemical properties, which enable thermodynamic *prediction*. Possible in the ideal case, assessment is commonly faced with an absence of thermochemical data due to the frequently unique chemical nature of the mineral phases newly formed during waste generation or stabilization (same structure, but anomalous element content, artificial structure). To compensate for this, many authors have

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turned towards data estimation related to mineralogy knowledge. Historically, these methods have been developed in particular for silicates and sulphosalts in relation to equilibrium modelling in geological environments [6]. However, references also exist for phosphates [9,17] and manganese [11]. Initially, the estimations were purely empirical, the sum of the free energy of oxides and hydroxides [5,10,12,13]. They were then refined by integrating steps that increase the weight of the structure in the estimation by considering the intrinsic free energy of the O^{2-}–M^{z+} [14, 15] bond, the correction of shifts related to excess binding energy for the mineral families [17] and also the crystallochemical environment of the element concerned [1,6,20]. Finally, in the most developed approach [18,19], the proposed model includes many crystallographic parameters intrinsic to the structure (smallest bond distance, cell volume and refraction indices, and presence or absence of oxygen bridges between sites and of hydrogen bond), quantification of the attraction–repulsion energy and the polarization energy involved in the bond. The ultimate aim of data acquisition (estimated or measured) is their consideration in predictive models constructed for scenarios established according to the projected use of mineral waste.

In conclusion, mineralogy through its different aspects, the knowledge accumulated, its analytical potential, and relationships existing between structure and physicochemical characteristics, opens up important perspectives for the field of waste management and stabilization. It should be included as an essential step in the certification of stabilization processes for toxic substances: only precise definition of the intrinsic nature of the pollutant (molecule type, degree of oxidation) and of the existing relationship with the mineral trap (nature of the bonding, location in the host lattice) will enable sound predictive management of the waste problem.

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