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Integrating Geochemical Models and Pitzer-Based Nitrate Thermodynamics to Quantify Soluble Salt Inventories in Tailings Storage Facility Foundation Soils

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Foundation soils beneath tailings storage facilities (TSFs) in arid environments can contain variable quantities of highly soluble minerals (halides, sulfates, and nitrates). Identification and quantification of these phases is important for physical stability and water-quality prediction. For example, dissolution of these minerals in soils under the infrastructure can result in differential settlement of embankments, creation of karst-related pipes, among other issues.

Quantification of these soluble phases in commercial laboratories can be challenging because of non-specific database selection, and inadequate sampling or sample preparation. Therefore, soluble salt contents can be underestimated, and mineralogical information in internal corporate databases may be biased.

In this work we present a method to quantify soluble salts in TSF foundation soil samples by combining geochemical tests with geochemical modelling using an extended Pitzer database (Fig. 1).

Mineralogy was determined by TIMA/XRD and provides the basis for reactive mineral estimations in soil samples. Inverse modelling of SFE leachates was done in PHREEQC. Multiple inverse models were obtained for each sample, and the reactive mineral assemblage that resulted in the lowest mass transfer was selected.

In parallel, direct modelling of kinetic tests (humid cells and columns) were also used to estimate reactive mineralogy. Direct models were implemented in PHREEQC using the Pitzer formulation to represent the reduced activity of ions in high-salinity leachates. Because nitrate is a major anion in the system, we extended the Pitzer database by adding NO_3^- and relevant solid phases (Na, K and Mg-nitrates). Temperature-dependent Pitzer interaction parameters obtained from the literature ([1], [2]) were converted from their original functional form into PHREEQC's polynomial representation through interpolation.

These model-derived reactive assemblages were then used to extrapolate mineralogy from chemical analyses (Cl, S, NO_3), taking advantage of better accuracy and higher number of measurements. The extrapolated mineralogy was the input of reactive transport models to predict water quality at the TSF scale.

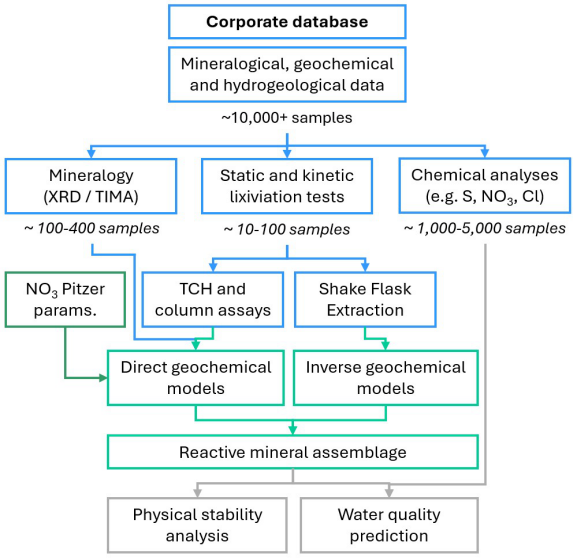

Figure 1: Method workflow

[1] Steiger, M. (2016), *Chemical Geology* 436, 84-97.

[2] Steiger, M., Kiekbusch, J., and Nicolai, A., (2006), *Construction and Building Materials* 22, 1841–1850.