

## Hydro-geochemical modeling in an artificial substrate: The legacy of bauxite refining

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In the bauxite refining Bayer's process, about 8 x  $10^7$  t/y of problematic residue is produced worldwide by extraction of alumina from bauxite earth. The bauxite refining industry requires strategies for rehabilitation of residue deposits to comply with legislation for site closure and to obviate future liability issues. A major challenge is the improvement of the chemical and hydrological conditions in bauxite residue to support sustainable vegetation cover for the purpose of dust suppression, leaching control and ecological functioning. Untreated bauxite residue impedes its use as a substrate for plant growth due to high pH (11-13), unfavorable nutrient status and low plant-available water content. Several minerals formed in the refining process are responsible for the longevity of this hostile environment, which affects water quality both in the saturated and unsaturated zone.

Geochemical modeling was used to build a clear understanding of the key processes occurring in untreated residue and, furthermore, to simulate the efficacy of engineered solutions such as amendment with gypsum and fertilizers aimed at improving the residue's pH and nutrient status. By means of modeling a sustainable rehabilitation and management strategy shall be elaborated, which shall then be tested under field conditions. The geochemical speciation code PHREEQC, which includes models for solid phase dissolution, cation exchange and surface complexation, was applied to study the consequences of calcium aluminum hydrates, zeolites and kaolinite as well as hydro-ferrous and aluminous oxides and organic acids in the artificial mineral mix. The combination of several geochemical sub-models and their evaluation allows prediction of the overall behavior of the soil solution in the substrate. Numerous generic column simulations were conducted to investigate the cation exchange properties of zeolites in the clay fraction and the buffering capacity of hydro-ferrous oxides. The results enabled critical assessment of the impact of gypsum amendment.