

Coupled hydrological and geochemical modelling of a tropical watershed

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Tropical areas cover about 40% of the continental surfaces. They contribute between 30% and 50% to the global discharge to the ocean. We propose to model weathering fluxes and associated CO₂ consumption at a catchment scale in this environment. In South India, the Western Ghats make an orogenic barrier to the SW monsoon. It induces a sharp climatic gradient, defining three climatic zones from the West to the East: humid, sub-humid and semi-arid zones. An experimental watershed, Moole Hole, is currently monitored in the sub-humid zone since 2003 (ORE-BVET).

Weathering fluxes are simulated with a lumped hydrological model coupled with a geochemical model of weathering process (WITCH). The model boundary conditions are defined from field hydrological, mineralogical and chemical data. The particular climate, alternating long dry periods with short but intense precipitation events, provides a good test for the robustness of the geochemical model.

The first step in this modelling is to properly calibrate the hydrological model with runoff measurements using precipitation and evapotranspiration data as input. The second step is to generate current soil solutions, groundwater and river chemical contents. Results are compared with field data on a three year measurement period. The coupled model evaluates the CO₂ consumption by weathering and its possible *in situ* carbon sequestration due to precipitation of pedogenic carbonates.

The coupling of hydrological and geochemical model offers the possibility to simulate scenarios of weathering under a varying climate. It can be used to explore the impact of man-induced global climate change on tropical weathering processes (monsoon precipitations are expected to increase when global climate is warmer).

A CD-MUSIC surface complexation database for modeling oxyanion sorption on Iron oxyhydroxides

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We have developed an internally consistent surface complexation reaction database for the sorption of As(III), As(V), B(III), Cr(VI), Mo(VI), S(VI), Sb(III), Sb(V), Se(IV), Se(VI), and V(V) on goethite and HFO based on the CD-MUSIC model. Surface complex geometries and reaction stoichiometries were constrained by spectroscopic studies where available. CD values (Δz_0 and Δz_1) for the surface complexes were obtained from published *ab initio* studies or estimated from bond valence principles. Iron oxide surface site densities of 3.45 and 2.7 sites/nm² were used for singly and triply coordinated >Fe sites, respectively, and inner and outer layer capacitances 0.85 and 0.75 F/m² were assumed.

Equilibrium constants for the surface complexation reactions were retrieved from an extensive experimental dataset of oxyanion sorption on goethite and HFO compiled from the literature through 2007.

The CD-MUSIC database provides a consistent, description of oxyanion sorption on iron oxyhydroxides over a wide range of pH, sorption site density, and solution composition, and is particularly useful for geochemical modeling of competitive sorption in multicomponent systems.

As ^{III}	>FeOAs(OH) ₂ , (>FeO) ₂ AsOH
As ^V	>FeOAsO ₃ H, (>FeO) ₂ AsO ₂ , (>FeO) ₂ AsO ₂ H
B ^{III}	>FeOB(OH) ₂ , >FeOB(OH) ₃
Cr ^{VI}	>FeOCrO ₃ , (>FeO) ₂ CrO ₂
Mo ^{VI}	>FeOMo(OH) ₅ , >FeOMoO ₃
S ^{VI}	>FeOSO ₃ , >FeOSO ₃ H, (>FeO) ₂ SO ₂ , (>FeO) ₂ SO ₂ H
Sb ^{III}	>FeOSb(OH) ₂ , (>FeO) ₂ SbOH
Sb ^V	>FeOSb(OH) ₅ , (>FeO) ₂ Sb(OH) ₄
Se ^{IV}	>FeOSeO ₂ , >FeOSeO ₂ H, (>FeO) ₂ SeO, (>FeO) ₂ SeOH
Se ^{VI}	>FeOSeO ₃ , >FeOH ₂ SeO ₄ , (>FeO) ₂ SeO ₂
V ^V	(>FeO) ₂ VO

Table 1: Surface complex stoichiometries.