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Kinetic Leaching Model for Arsenic in Soil: Bridging Soil Environments and Reactive Transport Models

BUM-JUN KIM AND MYOUNG-SOO KO
Kangwon National University

This study develops a kinetic leaching model for arsenic (As) in soil by incorporating soil characteristics and leaching conditions to enhance its applicability in reactive transport models (RTMs). The RTMs simulate element transport and geochemical reactions in aquifers and subsurface environments; however, they often lack thermodynamic data for As leaching in soil that limiting the models applicability to water-rock reaction. To address this, a kinetic leaching model was formulated to describe As extraction in soil under varying solution pH and reaction time, and subsequently integrated into RTMs. To evaluate pH-dependent As leaching kinetic rate, 1 g of mining soil samples were reacted with 5 mL of synthetic precipitation (pH 2.0–6.0) at 25°C. The solution was agitated at 35 rpm for 10–1080 minutes. The leaching data were fitted to the two-constant model, $C_t = A \cdot t^B$ (C_t: extracted As concentration, $\mu g \cdot kg^{-1}$; A: initial extraction rate constant, $\mu g \cdot kg^{-1} \cdot min^{-1}$; B: extraction coefficient). Pearson correlation and regression analyses showed that Factor *A* was strongly correlated with the concentration of mobile As (sum of non-specifically and specifically sorbed As in Wenzel's sequential extraction, F_m; r = 0.704, n = 247, p < 0.01) and influenced by solution pH. Factor *B* was expressed as a function of soil pH, indicating that lower B values at higher soil pH resulted from acid consumption by soil, which reduced the availability of H^+ for As extraction. These findings highlight that As mobility in natural environments is mainly controlled by mobile As (F_m) in soil and solution pH. Based on these statistical results, a quantitative kinetic model was formulated as Eq. (1). The derived kinetic leaching model was implemented in Geochemist's Workbench (REACT module) using a custom BASIC code and validated against 275 experimental results, yielding an RMSE of 3.1 and accurately predicting As leaching within the range of 0.01–80 mg/kg. Thus, by incorporating this kinetic leaching model, RTMs can more accurately simulate pH-dependent As extraction, overcoming limitations in thermodynamic data for As release from soil. This integration enhances predictions of geochemical element distributions, contamination risks, and remediation strategies in soil and water systems.

$$C_t\ (\mu g \cdot kg\text{-}1) = \exp\{0.88+0.02\ln(1000[H^+]) \cdot \ln(F_m)\} \times t^{0.001\exp\{5.5-0.4\ln(\text{soil pH})\}} \quad \text{Eq. (1)}$$