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Modeling dehalogenation of diatrizoate by sulfide-modified nano-scale zero-valent iron in natural porous media.

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Iodinated Contrast Media (ICM) are organic compounds, widely used during X-ray procedures for medical imaging [1]. ICM are connected with diseases, such as hyperthyroidism or hypothyroidism, due to the iodine ions bound to the chemical molecule [2]. Moreover, in aquifer system, ICM can form toxic intermediate products during photodegradation or Managed Aquifer Recharge processes [1].
Nano-scale zero-valent iron (nZVI) can efficiently dehalogenate ICM and turn ICM into non-toxic products [1]. The chemical reaction between ICM and nZVI is impacted by several factors, such as the initial concentration of nZVI, the presence of oxygen in the subsurface environment (i.e., the occurrence of anaerobic versus aerobic conditions) and the pH of fluid phase. Although several experimental studies have analyzed the reaction kinetics between ICM and nZVI at laboratory scale under batch conditions ([3],[4],[5]), few studies have investigated the interaction between ICM and nZVI under flow conditions. In this framework, Zhou et al. [6] performed both batch and column experiments in order to identify the reaction mechanism and kinetics of diatrozate (DTA) dehalogenation using sulfide-modified nZVI (S-nZVI) under anaerobic conditions. The authors also proposed a pseudo-first-order kinetic model to interpret the batch experiment outcomes. However, the proposed model cannot adequately reproduce the experimental results obtained under flow condition.
Here, we cast the batch experiment of Zhou et al. [6] within a stochastic framework and (i) provide Maximum Likelihood estimates and associated uncertainties of characteristic parameters driving the underlying kinetic mechanisms and (ii) assess the way uncertainty associated with model parameters propagates into uncertainty in quantifying the temporal evolution of DTA concentration. Finally, we propose a new kinetic model able to describe the interaction between DTA and S-nZVI under flow conditions. The new kinetic model which includes advective-dispersive transport, sorption and desorption to and from the reactive surface (S-nZVI), dehalogenation of DTA by S-nZVI, adequately reproduces the experimental results.

Participation

In-Person

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