

Targeting a safe aquifer in the Arsenic contaminated alluvial deposits

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The present study aims to investigate the sorption and mobility of As in the contaminated sediment-groundwater (GW) interface to find out a likely safe aquifer beneath the Holocene deposit. The results show that the deeper sediment (> 100 m) comprising of partly oxidized, brownish medium sand (As, 0.76 µg/g) that accommodates much natural adsorbing surfaces like Fe and Al, was found to provide considerably low As (4 µg/L) water. A relatively faster *in situ* reaction rate, K_r (2.72×10^{-16} /sec) derived by using inverse mass balance model could also enhance the essential As releasing process from the upper source sediment. The distribution of As in the sediment-water interface was recognized by computing a partition coefficient, K_d -As by employing *in situ*, batch adsorption and flow through column techniques separately and was found to vary ranging between 10 and 250 L/kg. Additionally, a parametric equation to predict that K_d -As ($R^2 = 0.67$) was postulated from the GW-pH and logarithm of leachable Fe and Al contents in sediments. Incorporating these K_d and K_r , a 1-D finite difference numerical model was applied which showed that even after 80 years (Fig.1) not only the upper leached As could be immobilized against reaching the deeper aquifer due to the presence of a natural filter (oxidizing sand and adsorbing minerals Fe, Al), but also much of its GW As (83%) might get reduced. Finally, the deeper aquifer could be considered as the sustainable source of safe and adequate water to meet the urgent demand.

Figure 1: Prediction of As scenario after 80 years

Towards accurate modeling of the growth and nucleation of carbonates

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The nucleation and growth of CaCO₃ is of significant interest in a number of fields, including biomineralization. In order to understand the atomic detail of how such processes occur, it is valuable to perform computer simulations alongside experimental studies. Our ability to perform accurate dynamical simulations of the aqueous CaCO₃ system is hindered by two aspects. Firstly, the challenge of correctly describing the phase diagram of calcium carbonate; it is well known that the competition between calcite, aragonite, vaterite and amorphous precursors is very sensitive to particle size and conditions. Secondly, there is the issue of speciation; when does the interconversion between bicarbonate and carbonate occur and how does this influence growth processes?

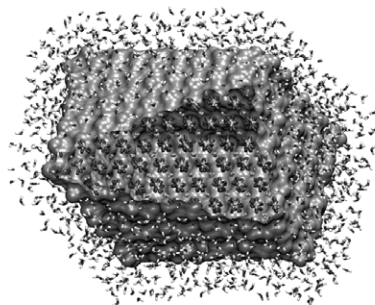


Figure 1: Solvated nanoparticle of CaCO₃.

In this study we propose new force-field based methods [1] to address both of the above problems, thereby offering a route towards the accurate simulation of this system. To illustrate this, results for the properties of CaCO₃ nanoparticles in water (Figure 1) will be presented.

[1] Raiteri *et al.* (2010) *J. Phys. Chem. C*, in press.