Numerical simulations (COMSOL) of γ-Fe_2O_3 nanohybrids for transport (3D) and arsenic removal in homogeneous porous media

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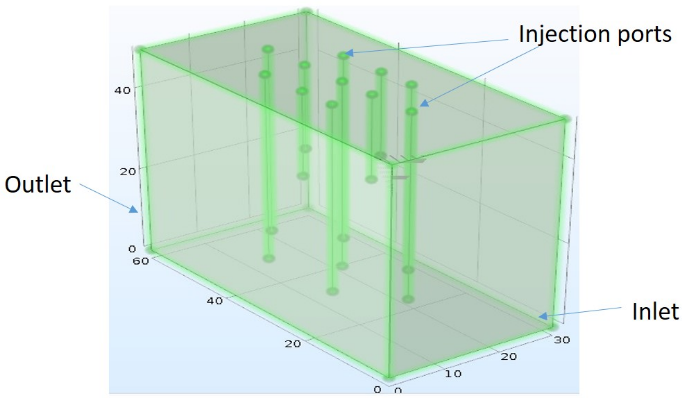
Worldwide, arsenic is a menace among the living communities due to its contamination in groundwater. It leaches moderately into groundwater from earth crust and bedrocks enriched with its ores. The countries like India and Bangladesh are being critically affected due to their densely populated areas. Several nanomaterials have been developed and examined as adsorbents for its removal, which are being utilized in *ex-situ* remediation technique. This technique has the disadvantages in terms of generating highly toxic waste, causes due to its easy mobilization in the living ecosystems. Nowadays, *in-situ* (subterranean) sequestration of arsenic is gaining considerable attention in respect to reduce the chance of its mobilization in living environment.

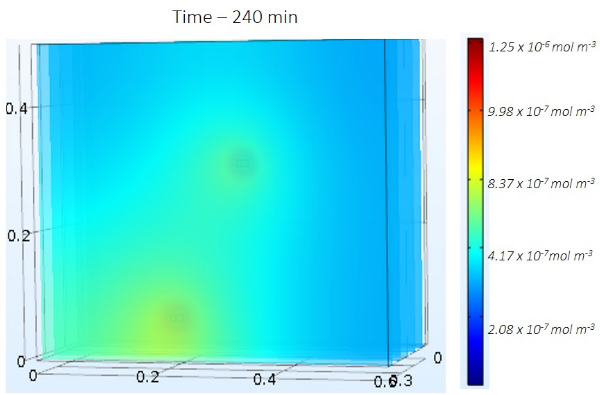
To this aim, the γ-Fe_2O_3 nanohybrids are developed using a novel approach of synthesis which include the usage of industry waste as one of precursor material. These nanoparticles have been found significantly stable in aqueous solutions representing real world groundwater conditions. The measured zeta (ζ)-potential value of -31.6 mV, indicated their significant colloidal stability. In respect to *in-situ* application, the understanding of transport modeling and retardation of nanomaterials in aquifer systems by simulating through numerical models in complex 3-dimensional scenario are necessary. Therefore, a modeling approach based on modified advection-dispersion-retardation equations has been investigated, considering the coupled influence of head difference and reaction rate of particle transport.

All the experiments were performed in a sand-tank set up (0.6 x 0.3 x 0.50 m) having several injection ports at variable depths. The tank was packed with the porous media (medium size sand) having the grain size (mm), grain density (g cm^{-3}), bulk density (g cm^{-3}) and effective porosity (%) values of 0.5-1.0, 2.33 ± 0.2, 1.55 ±0.09 and 0.34 ±0.1, respectively. The longitudinal and traverse dispersivity of consolidated media were calculated using NaCl as a tracer. The COMSOL Multiphysics model (subsurface module) was investigated for simulation of γ-Fe_2O_3 nanohybrids injection and their transport through porous media. Transport of arsenic and as-synthesized nanomaterial were modelled by considering these as solute and colloid, respectively, under fully saturated homogenous porous media and variable flow rate conditions. After simulation, the colloidal solution of nanoparticles was allowed to inject at the concentration of 1.25 x 10^{-4} mol m^{-3} and flow rate of 1.2 L h^{-1}. The simulation results were matched with the experimental observations which provided estimates of transport parameters. The retardation efficiency utilized to predict the γ-Fe_2O_3 nanohybrids in similar porous media, although the extend of injection pressure, colloid concentration and pumping rate may be underpredicted which require further investigations.

Keywords: Numerical modeling, In-situ arsenic sequestration, Groundwater



3-Dimesional view of Sand-Tank set up



Transport of nanohybrids (Simulation)