INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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The conventional computational models on solute transport use the simple advection diffusion equation to simulate the contaminant movement in subsurface, however, the equation has some limitations since some processes cannot be simulated; like occurrence of non-equilibrium in mass distribution during transport through the porous medium. This happens due to the presence of stagnant (immobile) water at the disconnected pores (dead end pores) of porous medium, where the velocity of the stagnant water is negligible with respect to mobile water. Mass transfer happens due to the physical nature of soil is defined as physical non-equilibrium. Mass transfer between mobile and immobile water region retards the contaminant transport and the immobile water zones may act as sinks/sources of contaminants and it can cause non-ideal conditions in solute distribution and early arrival of solutes at the downstream. Contaminants like Acid Mine Drainage (AMD), effluent acidic water that drains from the mining sites, etc. are reactive in nature and it will be interesting to study the transport of AMD in the presence of non-equilibrium mass transfer. Pyrite oxidation reaction adds acidity to the surface water that leads to the dissolution of heavy metals and its transport towards groundwater zone. This research conceptualizes the liquid zones in the porous subsurface medium to have mobile and immobile zones. In addition, the study emphasizes the use of mass transfer of water as well as contaminants simultaneously between the mobile and immobile regions that are rarely studied. The open source FEMWATER model, developed by USEPA, was modified to accommodate liquid mass transfer between the mobile and immobile regions and the transport module, 3DLEWASTE, was modified to handle the non-equilibrium solute mass transport and an ion-exchange reaction is newly added to the source code of the model. Modified model was applied to the hypothetical domain to study the reactive transport under various conditions: i) homogeneous and heterogeneous domain, ii) conservative and reactive transport, iii) equilibrium and non-equilibrium transport. Difference in contaminant (ferrous ion) spreading patterns are observed between the advection-dispersion model and physical non-equilibrium models, which is evident from the advancement of the solute front in the direction of water flow. A difference in contaminant spreading pattern is also observed between first and second type non-equilibrium models. In conventional physical non-equilibrium transport models (first type non-equilibrium), the water content value is split between mobile and immobile water contents. Second type non-equilibrium model, where time dependent water transfer is considered, simulates natural mass transfer process unlike the first type model, which properly could not capture the velocity details of mobile-immobile flow. Little difference is observed in the contaminant spreading pattern between homogeneous and heterogeneous domain simulations, especially for the contaminant in the immobile water zone. Though sorption and ion-exchange reactions limit the contaminant transport in subsurface region, mobile-immobile flow advances the solute front. In the case of reactive transport, compared to sorption, the ion-exchange reaction is less affected by the non-equilibrium process. There are mainly two parameters i) ratio of mobile water content to total water content (f) and ii) mass transfer rate constant (Γ), which affects the contaminant transport properties, especially a high immobile water content causes a quick arrival of solute front at the downstream boundary.