Fate and Transport Study of Contaminant through Saturated Porous Media

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Declaration by the Research Scholar

I hereby declare that the entire work embodied in this Thesis entitled "**Fate and Transport Study of Contaminant through Saturated Porous Media**" is the result of investigations carried out by me in the **School of Engineering**, Indian Institute of Technology Mandi, under the supervision of **Dr. Deepak Swami**, and that it has not been submitted elsewhere for any degree or diploma. In keeping with the general practice, due acknowledgments have been made wherever the work described is based on finding of other investigators.

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Declaration by the Research Advisor

I hereby certify that the entire work in this Thesis has been carried out by **Abhimanyu**, under my supervision in the **School of Engineering**, Indian Institute of Technology Mandi, and that no part of it has been submitted elsewhere for any Degree or Diploma. In keeping with the general practice, due acknowledgements have been made wherever the work described is based on finding of other investigators.

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Abstract

Groundwater is an important source of the fresh water, as in most of the cases it is readily potable, due to natural filtration processes. It consists of a 30.1 % of the world's freshwater resources. Considering the recent water resources crisis due to exponential increase in the world's population, pertaining anthropogenic activities and urbanization, it becomes essential for water resources planning and groundwater plays a pivotal role in that. For an effective water resources planning, understanding the associated complexities with the groundwater is important. Nonlinear distribution of soil particles of different sizes and textures attributes to the heterogeneity. The release of the various chemicals due to natural and anthropogenic activities adds up the complexities in groundwater planning.

Various studies are conducted to model contamination transport through groundwater that employed computational techniques. Non-equilibrium conditions significantly influence the solute fate. The soil consists of multiple porosity regions popularly divided in macro-meso-micro scales. Most of the time flow takes place from primary and secondary porosities i.e. macro and meso. Due to the well-connected pores in these zones, contaminant can travel significant distances and pollute the groundwater. The tertiary porosity zones (micro-pore) do not participate in the flow directly, but due to the hydraulic connectivity, they store and release the contaminants in the flowing zones by diffusive gradient. The present study considers non-equilibrium and addresses the complex processes associated with possible solutions.

Therefore the first chapter of the thesis highlights the non-fickian behavior of the dynamic diffusive gradient developed during the transport of any solute (reactive or nonreactive). To incorporate the physical processes based on these flow preferences, REV is partitioned as macro-micro porosities which is knowns as dual porosity or mobile-immobile model. For a time-dependent solute source, BTC's consists of two parts i.e. rising and falling limbs. During rising part, the concentration in mobile region is higher and mass transfer occurs from mobile to immobile region. However, during falling limb concentration in immobile region tend to have higher values, resulting in reverse diffusive mass transfer process. That leads to the first objective of the thesis to develop the solution to overcome the reported limitation of mobile immobile model (MIM) in prediction of long tails of BTC during falling limb.

An approach is proposed that is based on dynamics of time resident concentration and its gradient between hydraulically coupled mobile and immobile regions. In this modified MIM, we estimated two distinct diffusive MTCs for rising and falling limb (RFMT) of BTC's using non-linear least square optimization algorithm. Two experimental data set from literature are simulated using numerical solution of proposed model and asymptotic time dependent dispersion function. Estimated parameters supported the hypothesis that for pulse type input, liquid phase transport during rising limb of BTC's is governed by advection and dispersion, whereas during falling limb it is majorly diffusive dominated that can be represented by the new MTCs. Simulated results of RFMT are then compared with constant mass transfer (CMT) approach to compare the quality of simulation. Sensitivity analysis is also carried out to evaluate the capabilities of RFMT over the rising and falling portions of BTC's. The study reveals that the concentration difference between the hydraulically connected regions (Mobile-Immobile) is temporally variable, as the concentration stored in the distributed immobile region becomes higher than mobile region when the source at inlet is completely consumed.

The limitation of the model based on dual porosities is that once the solute drives in to the matrix, it will further move across the transverse direction due to the diffusive gradient only. That is because zones of secondary porosities are not considered. Therefore the due attention to the flow in the secondary (meso) pore structures is given. To fulfil the second objective, a conceptual model of triple porosity non-equilibrium (TPNE) that accounts for physical and chemical non-equilibrium to describe the reactive solute transport through macro-meso-micro porosities is developed. Third objective of the thesis presents the details of semi-analytical solution of TPNE model derived in the Laplace domain and then numerically inverted in time domain to calculate the concentration in the porous medium. The model can accommodate semi-infinite extent of the porous medium. The present semi-analytical solution have been validated with existing analytical solution for heterogeneous porous medium. The fourth objective is to carry out temporal moment analysis in order to quantify the effects of mass transfer, sorption and other transport related parameters. In addition, the sensitivity of the model parameters and response of the breakthrough curves is also studied. An insight to the intra and inter-aggregate sorption and mass transfer processes is also discussed. The fifth and final objective of the thesis is to demonstrate the capabilities of TPNE model to simulate the experimental BTC's. It is observed that the TPNE model can well simulate the experimental datasets compared to the models based on dual porosity or dual permeability with first order kinetics and mass transfer processes. Since the TPNE model takes into account detailed sorption and mass transfer dynamics it is suitable for process level investigation. From the statistical measures (Akaike information criteria) it is demonstrated that use of T.P.N.E. is extremely useful and detailed as compared to the models based on dual porosity.

The thesis concludes that a single mass transfer approach for a thick immobile region underestimates the mass distribution in tailing region, therefore RFMT approach is more suitable if modeller wish to use MIM. Alternatively, if sufficient parameters are available, proposed semi-analytical solution of TPNE model can be used for detailed investigation of the fate of solute through heterogeneous porous medium.

Keywords: *concentration gradient, diffusive mass transfer, rising and falling limb, triple porosity, non-equilibrium, semi-analytical solution, temporal moments.*

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