Solute Transport Modelling through Saturated Porous Media with Time-dependent Dispersion

A THESIS

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Abhay (Roll No. S15004)

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Declaration by the Research Scholar

This is certify that the Thesis entitled **"Solute Transport Modelling through Saturated Porous Media with Time-dependent Dispersion",** submitted by me to the Indian Institute of Technology Mandi for the award of the Degree of Master of Science (by research) is a bonafide record of research work carried out by me under the supervision of ***Dr. Deepak Swami (Advisor)*** *and* ***Dr. Dericks Praise Shukla (Co-Advisor)*****.** The content of this Thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any Degree or Diploma**.**

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Declaration by the Research Advisor

This is certify that the Thesis entitled **"Solute Transport Modelling through Saturated Porous Media with Time-dependent Dispersion",** submitted by ***Abhay*** to the Indian Institute of Technology Mandi for the award of the Degree of Master of Science (by research) is a bonafide record of research work carried out by him under our supervision. The content of this Thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any Degree or Diploma.

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ABSTRACT

Groundwater is considered as the major source to meet the requirements of various demands, such as agricultural, domestic and industrial use. The movement of groundwater is slower as compared to the surface water which makes it more susceptible to pollution. Solute (contaminant) transport through soil (porous media) has been an important area of research for decades in the field of geo-environmental engineering. There are numerous sources that can contaminate soil and groundwater e.g. migration of leachate from dumping site, release of chemicals from mining operations such as tailing ponds. Contaminants when released into the environment, their transport occurs in the saturated groundwater zone as they infiltrate beyond the vadose zone. These contaminants cause pollution by interacting with water and soil at physical, chemical and hydrological domains. Thus, it becomes important to understand the transport mechanism of solute through saturated porous media so that the health risk can be avoided by detecting, simulating and predicting the movement of contaminant along with the groundwater. Solute transport in soil and groundwater is governed by various physical, chemical and biological process that takes place between solute and porous media. Advective transport with the flowing groundwater, mechanical dispersion due to heterogeneity of porous media, molecular diffusion, decay processes and equilibrium and non-equilibrium solute exchange with the solid phase are some of the well-known processes which govern the solute transport through porous media. All these processes play an important role in plume spreading and dilution, therefore quantification of impact of these processes on solute transport is essential to ensure the optimal cleaning operations. Most challenging task is to accurately predict the arrival time and spatial patterns of contaminant plume in the subsurface environment. The difficulty in prediction increases with the heterogeneity and chemical properties of solute and porous media. When solute transport parameters are different at different spatial and temporal scale, then predicting the behavior of solute in porous media become difficult.

There are numerous studies that utilize numerical modelling technique to study the contaminant behaviour in heterogeneous porous media. It has been reported in literature that the dispersion phenomenon affects the plume behaviour in porous media. Influence of scale (distance) - or time-dependent dispersion on solute transport has been observed at various scales. Therefore, present study focuses on the development of solute transport model which incorporate time-dependent

dispersion with physical partitioning of heterogeneous porous media. Physical non-equilibrium is accounted by diffusive mass transfer between mobile and immobile regions partitioning within the porous medium.

In this study, hybrid numerical solution of the mobile-immobile model (MIM) with linear and asymptotic time-dependent dispersion has been presented to account for heterogeneity of porous media. Observed data of solute transport through heterogeneous porous media (heterogeneous soil column and hydraulically coupled stratified porous media) has been simulated using constant, linear and asymptotic time-dependent dispersion models. To compare the simulation capabilities of transport models, results of timescale breakthrough curves and temporal moments have been compared between constant and time-dependent dispersion models.

Analysis of simulated breakthrough curves suggested that the system is under the strong influence of physical nonequilibrium which is evident by variable mass transfer coefficient estimated at different down-gradient distances. Non-Gaussian breakthrough curves comprising long tails are simulated well with the MIM incorporating asymptotic time-dependent dispersion model. Asymptotic dispersion function is found to be capable of capturing the rising limb of the solution phase breakthrough curves with improved accuracy, whereas tailing part simulation capabilities were similar for both asymptotic and linear time-dependent dispersion functions.

Further, the study deals with the estimation of solute transport parameters in saturated porous media with time-dependent dispersion models. Inverse parameter estimation procedure has been developed by coupling finite difference based solute transport model with the Levenberg-Marquardt algorithm. It is observed that the optimization algorithm results in non-unique optimal estimates for the case of more than three unknown parameter estimation with asymptotic time-dependent dispersion model. Asymptotic time-dependent dispersion model results in less number of non-unique optimal estimate parameters combinations in comparison to linear time-dependent dispersion model. Optimization algorithm resulted in non-unique estimates for asymptotic dispersion model in the case of simultaneous estimation of two or more unknown parameters. This is due to presence of equilibrium sorption coefficients of mobile and immobile region. Finally, inverse algorithm is utilized to estimate unknown transport parameters from a column experiment data of conservative solute and it is concluded that the asymptotic time-dependent dispersion model fits the observed data much better than linear time-dependent dispersion model.

In the end, temporal moment analysis is presented to study solute plume behavior and sensitivity of time-dependent transport parameters. Temporal moment analysis revealed that the solute mass recovery, mean residence time and variance of breakthrough curve are sensitive to the estimated parameters. It also revealed the limitation of MIML at higher travel distances and endorsed the use of MIMA for field applications due to its realistic representation of spreading, skewness and mean travel time of solute plume. Zeroth temporal moment for MIMA model attains an asymptotic value as the plume travel distance increases within porous medium while for MIML it keeps on decreasing. The pattern of the first moment reveals the physical ever-growing nature of the MIML model which tends to demonstrate nonrealistic representation of the plume behavior without any upper bound. It can be concluded from the study that MIM with asymptotic time-dependent dispersion function is a simpler yet powerful tool to account for medium's heterogeneity.

Keywords*:* Solute transport, Mobile-immobile model, Time-dependent dispersion, Parameter estimation, Temporal moments.

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