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A Layer-Integrated Model of Solute Transport in Heterogeneous Media

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Abstract. This study presents a numerical solution to the three-dimensional solute transport in heterogeneous media by using a layer-integrated approach. Omitting vertical spatial variation of soil and hydraulic properties within each layer, a three-dimensional solute transport can be simplified as a quasi-three-dimensional solute transport which couples a horizontal two-dimensional simulation and a vertical one-dimensional computation. The finite analytic numerical method was used to discretize the derived two-dimensional governing equation. A quadratic function was used to approximate the vertical one-dimensional concentration distribution in the layer to ensure the continuity of concentration and flux at the interface between the adjacent layers. By integration over each layer, a set of system of equations can be generated for a single column of vertical cells and solved numerically to give the vertical solute concentration profile. The solute concentration field was then obtained by solving all columns of vertical cells to achieve convergence with the iterative solution procedure. The proposed model was verified through examples from the published literatures including four verifications in terms of analytical and experimental cases. Comparison of simulation results indicates that the proposed model satisfies the solute concentration profiles obtained from experiments in time and space.

AMS subject classifications: 65C20, 65M99

Key words: Layer-integrated model, groundwater, solute transport, finite analytic method, heterogeneous media.

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1 Introduction

The major difficulty of groundwater solute transport simulation could be attributed to the large degree of heterogeneity in the subsurface. In reality, physical properties of subsurface porous media are spatially and temporally variable rather than homogeneous, and could be simply considered as a multi-layered system. Therefore, groundwater solute transport simulation is usually performed by employing the concept of multi-layered system if the spatial variability of soil and hydraulic properties can be negligible within each layer and the subsurface porous media can be assumed as a series of parallel homogeneous layers with finite thickness. In the past decades, a number of analytical or semi-analytical solutions to solute transport in multi-layered system have been developed by many investigators, including one-dimensional diffusion modeling [3, 19], one-dimensional advection-diffusion modeling [4, 11, 13, 17, 18] and two-dimensional advection-diffusion modeling [1,24,30,31].

Although, analytical solutions are free from numerical dispersion and other truncation errors that are often observed in numerical simulations, the initial and boundary conditions are so limited that are not suitable for many practical problems. Therefore numerical methodology is more widely applied, and consequently a variety of numerical schemes, as reviewed by Zhao et al. [32], have been developed. On the other hand, a fully three-dimensional model, which can appropriately simulate the aforementioned solute transport, may be overwhelmed by the demand of a large number of nodes or elements to become impractical to solve. To overcome these disadvantages, some researchers introduced a multi-layered technique to simplify the three-dimensional computation processes by splitting the entire domain into a number of thin layers. The full three-dimensional simulation can be reduced to the combination of vertical one-dimensional and horizontal two-dimensional computations. It would disregard some noticed local features but significantly reduces the consumption of computational time to improve feasibility and practicability. This conceptual procedure was first used in coastal water simulation [7, 10, 12, 14] and was later adopted and applied in some fields such as open-channel flow applications [5,9,21,28] and subsurface flow simulation [15,22,29]. A similar concept was also used to examine groundwater solute transport in heterogeneous media [8], where a hybrid model was constructed by applying the finite analytic method for the horizontal two-dimensional computation along with an analytical function for the vertical one-dimensional computation. Through a multi-layered procedure, the model is suitable for large-scale simulation and demonstrates both accuracy and efficiency compared with analytical solutions.

The purpose of this paper is to test the feasibility of the latter approach. A quasi-three-dimensional numerical model, based on the multi-layered technique, is proposed to deal with this subject. The fundamental concept of the adopted approach is similar to Kuo et al. [8], but we solve the vertical solute profile numerically by introducing a quadratic function instead of using an analytical solution. The newly-proposed model can relieve the limitation of Dirichlet type boundary conditions along the upper boundary and Neu-