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Contaminant Transport Modeling through Saturated Porous Media Using Finite Difference and Finite Element Methods

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ABSTRACT: *This paper presents an alternative numerical method to model the two dimensional contaminant transport through saturated porous media using a finite difference method (FDM) and finite element method (FEM). A finite-difference model is constructed by dividing the model domain into square and rectangular regions called blocks or cells. Concentrations are computed at discrete points within the model called nodes. The network of cells and nodes is called the grid or mesh. For analysis, the two-dimensional advection-dispersion equation with sorption is considered. MATLAB code is developed to obtain the numerical solution. CTRAN/W is also used for modeling of contaminant transport which is based on the finite element method. Results of the FDM and FEM are compared and it is found that they agree well.*

Keywords: *Advection, Finite Difference Method, Finite Element Method, Saturated Porous Media.*

I. INTRODUCTION

For a proper assessment and management of groundwater resources, a thorough understanding of the complexity of its processes is quite essential. Expansion of human activities causes dispersion of pollutants in the subsurface environment. The fate and movement of dissolvedsubstances in soils and groundwater has generated considerable interest out of concern for the quality of the subsurface environment. Groundwater flow and transport analysis have been an important research topic in the last three decades. This is due to the fact that many of the geoenvironmental engineeringproblems have direct or indirect impact on the groundwater flow and solute transport. Solute transport by flowing water (dissolved suspended particles) has broad impact in environmental protection andresource utilization via groundwater contamination. The leaching (displacement) of salts and nutrientsin soils also has an impact on agricultural production [1].

In the present investigation, an attempt has been made to provide a simple but sufficiently accurate methodology for numerical simulation of the two-dimensional contaminant transport through the saturated homogeneous porous media and landfill liners using finite difference and finite element methods. The physical processes such as advection, dispersion, and diffusion and interaction between the solution and the soil solids such as sorption, biodegradation, and retention processes have been considered in the governing equation used in the present study. Finite difference method has been adopted herein to solve the two-dimensional contaminant transport equation to predict the pollutant migration through soil in waste landfill. In the finite difference technique, the velocityfield is first determined within a hydrologic system, and these velocities are then used to calculate the rate of contaminant migration by solvingthe governing equation. A MATLAB code is developed for the finite difference method to obtain the numerical solution.

Finite element method is also used to model the contaminant transport through the porous media using Geostudio/CTRAN-W software. Results of the finite difference method (FDM) are compared with those obtained from thefinite element method (FEM). The FDM has generated the stable and convergent results for the advection-dispersion-sorption problems.

II. Mathematical Model

Mathematical models are used in simulating the components of the conceptual model andcomprise an equation or a set of governing equations representing the processes that occur,for example groundwater flow, solute transport, etc.The differential equations are developed for analyzing the groundwater flow (and transport)and are known to govern the physics of flow (and transport). The reliability of modelpredictions depends on how well the model approximates the actual natural situation in the*field*. Simplifying assumptions are made inorder to construct a mathematical model, because the field situations are usually too complex to simulate exactly[1].

Mathematical models of groundwater flow and solute transport can be solved generally with two broad approaches:

Analytical solution of the mathematical equation gives *exact* solution to the problem, i.e., the unknown variable is solved continuously for every point in space (steady-state flow and time (transient flow).Analytical models are exact solution to a specified, well simplified groundwater flow or transport equation. Because of the complexity of the three-dimensional (3D) groundwater flow and transport equations, the simplicity inherent in analytical model makes it impossible to account for variations in field conditions that occur with time and space. For these problems, (variations in field conditions) such as changes in the rate/direction of groundwater flow, stresses, changes in hydraulic, chemical and complex hydrogeologic boundary conditions, the assumptions are to be made to obtain an analytical solution which is far way from the reality. To solve mathematical models of this nature, one must resort to approximate methods using numerical solution techniques.

Numerical solution of the mathematical equation gives *approximate* solution to the problem, i.e., the unknown variable is solved at discrete points in space (steady-state flow) and time (transient flow). Numerical models are able to solve the more complex equations of multidimensional groundwater flow and solute transport. Many numerical solutions to the advection-dispersion equation have been reported (Fig 1). The most popular techniques are as the Finite Difference Method and Finite Element Method.

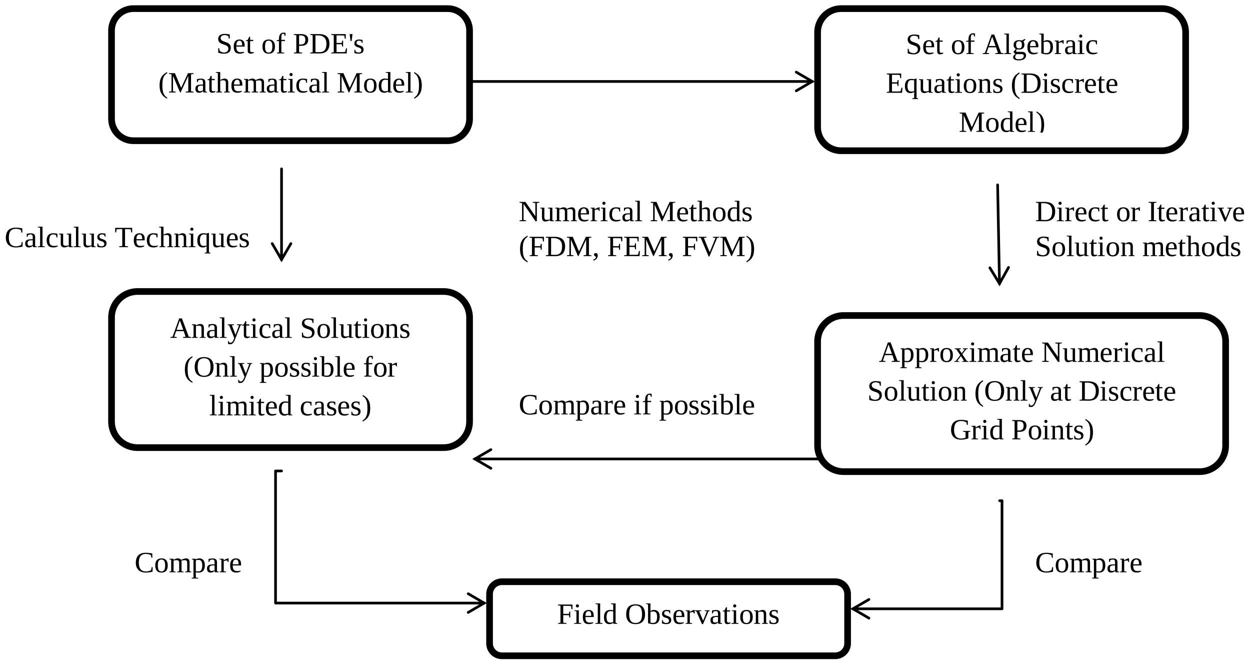


Fig 1: Flow chart showing the approach to mathematical model solutions [1]

III. CONTAMINANT (SOLUTE) TRANSPORT EQUATION

The transport of solutes in the saturated zone is governed by the advection-dispersionequation which for a porous medium with uniform porosity distribution is formulated asfollows

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial xt}(cvi) + \frac{\partial}{\partial xi}\left[Dij\frac{\partial c}{\partial xj}\right] + Rc \qquad i, j = 1, 2, 3 \qquad (1)$$

Where
∂ = delta function meaning change in;
x = the dimension (m);
t = the time (s)
c = concentration of the solute (kg/m^3);
Rc = reaction rate (concentration of solute) in the source or sink ($kg\ m^3/s$);
Dij = dispersion coefficient tensor (m^2/s);
vi = velocity tensor (m/s).

An understanding of these equations and their associated boundary and initial conditions is necessary before a modelling problem can be formulated.

From above equation, the first term on the right hand side represents advection transport and describes movement of solutes at the average seepage velocity of the flowing groundwater.The second term represents the change in concentration due to hydrodynamic dispersion.The third term represents the effects of mixing with a source fluid of different concentration from the groundwater at the point of recharge or injection [2].

The solute transport (advection-dispersion) governing equation based onthe assumption that the reactions are limited to equilibrium-controlled sorption. The solution to this governing equation is identical to the solution for the governing equation without sorption effects, except the velocity, dispersive flux and source are deduced by the retardation factor "R". The governing equation is as follows

$$R\frac{\partial c}{\partial t} = -\frac{\partial}{\partial xt}(cvi) + \frac{\partial}{\partial xt}\left[Dij\frac{\partial c}{\partial xj}\right] + \frac{Rc}{S} - R\lambda c \qquad (2)$$

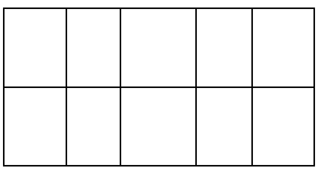
IV. Finite Difference Method

The partial differential equation describing the flow and transport processes in groundwaterinclude terms representing derivatives of continuous variables. Finite difference method isbased on the approximations of these derivatives (slopes or curves) by discrete linear changes over small discrete intervals of space and time. A situation where the intervals areadequately small, then all of the linear increment will represent a good approximation of the true curvilinear surface [1].

Finite difference mesh

A finite-difference model is constructed by dividing the model domain into square orrectangular regions called blocks or cells. Head, drawdown, and concentration are computed at discrete points within the model called nodes. The network of cells and nodesis called the grid or mesh.There are two main types of finite difference techniques, known as block-centered and mesh-centered. The name of the technique refers to the relationship of the node to the grid lines. Head is computed at the center of the rectangular cell in the block-centered approach. Conversely, head is computed at the intersection of grid lines (the mesh) in the mesh-centered technique. Fig 2 illustrates this concept graphically.

1 2 3 4 5 6
COLUMNS



ROWS

1 2 3 4 5 6

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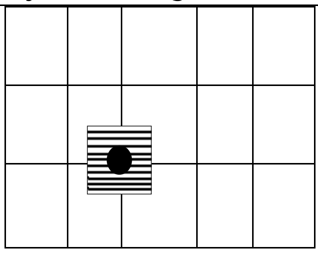

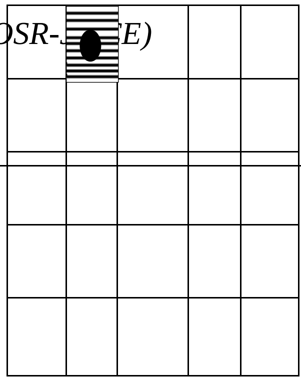

MESH- CENTERED BLOCK- CENTERED

Node Area of Influence

Fig 2: The finite difference grid

V. NUMERICAL EXAMPLE : RESULTS

Table 1 gives the parameters considered for thenumerical example. The problem domain isshown in Fig3. In this case, the simulation has been carried out for 630 days with a time step of 15 days.In the finite element analysis, the domain is discretised into 4-noded 307 elements with 342 nodes. A comparison between the concentration profilesobtained from the FDM and FEM for advection-dispersion-sorption case for the differenttime periods made. Fig 4 depicts the concentration contours obtainedfrom the FEM and FDM for three different time periods.

Table 1 Data Used for Advection-Dispersion-Sorption [3]

Parameter	**Value**
Seepage velocity (m/day)	0.864
Length of the reach (m)	80
Width of the reach (m)	80
Longitudinal dispersivity (m)	1.75
Transverse dispersivity (m)	1.75
Retardation factor	7.2674
Total duration of simulation (days)	630
Time step (Δt) (days)	20
Number of divisions in length direction	20
Number of divisions in width direction	20
Initial concentration (g/m^3)	0
Concentration at source boundary (g/m^3)	1.0

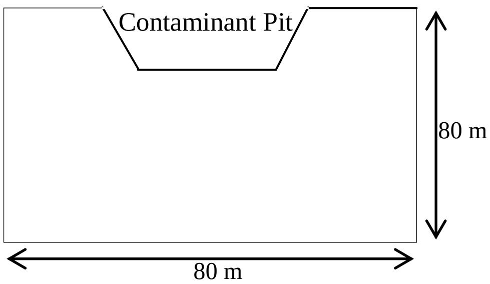

Fig 3: Sketch of problem domain

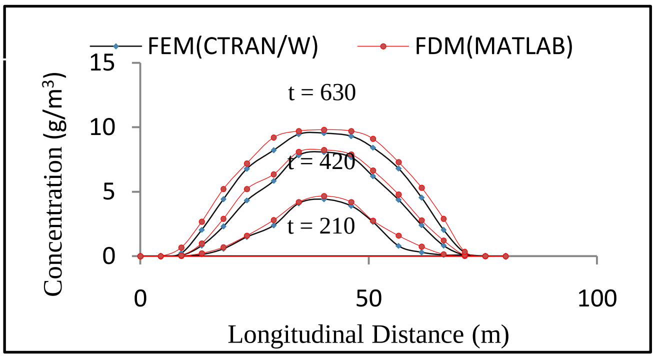

Fig 4: Concentration profile for different time periods (in days)

VI. CONCLUSIONS

Finite difference method is presented for modelling the two-dimensional contaminant transport through the saturated porous media. It is noted that the FDM is very simple and easy to implement irrespective of size and shape of the problem domain. From Fig 4, it is noted that both the finite difference and finite element results are matching well, thus ensures the correct formulation of the FDM for modelling of the two-dimensional contaminant transport process. The numerical methods like FEM and FDM allow solving the governing equation in more than one dimension.Most analytical solutions fail to provide acceptable results in the case of complex boundary conditions and for heterogeneous and anisotropic aquifers. In such cases, numerical solutions will provide a better alternative to the modelling of contaminant transport through porous media.

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