

Finite Element Method of Modeling Solute Transport in Groundwater Flow.

M.U. Igboekwe, Ph.D.

Department of Physics, Michael Okpara University of Agriculture, Umudike, Abia State, Nigeria.

E-mail: igboekwemu@yahoo.com

ABSTRACT

This study is undertaken to examine the movement of water solute from the surface of the Earth to the aquifer and also to assess the impact of existing or proposed activity on the quality and quantity of groundwater through the use of groundwater flow and solute transport models. Analysis was done using finite element method of Numerical Analysis (also known as finite element analysis) which is a numerical technique for finding approximate solutions of partial differential equations as well as that of integral equations. The solution approach is based on either eliminating the differential equation completely or rendering the partial differential equation into an approximating system of ordinary differential equation. This is then numerically integrated using standard techniques. The work thus involves the sub-division of the aquifer region into finite elements, in which a finite model is developed. This was then used to calculate the solute concentrations at different nodes in the divided continuum.

(Keywords: finite element method, continuum, groundwater, numerical analysis, solute transport, partial differential equation, aquifer)

INTRODUCTION

Groundwater refers to all the water occupying the voids, pores and fissures within geological formations which originated from atmospheric precipitation either directly by rainfall infiltration or indirectly from rivers, lakes or canals. Sands, gravel, sandstones, and limestone formations are the usual sources of groundwater supply though some may be drawn from impervious rocks such as granite when they have an over burden of sand or gravel (Olumuyiwa et al., 2012).

Groundwater is a valued fresh water resource and constitutes about two-third of the fresh water

reserves of the world (Chilton, 1992). Buchanan (1983) also estimated the groundwater reservoir of the world at about 5×10^{24} litres. This volume is more than 2,000 times the volume of waters in all the world's rivers and more than 30 times the volume contained in all the world's fresh water lakes. Groundwater is used for agricultural, industrial and domestic purposes. It accounts for about 50% of livestock and irrigation usage and just under 40% of water supplies, whilst in rural areas, 98% of domestic water use is from groundwater (Todd, 1980).

Utilization of groundwater as a source for domestic, municipal, agricultural and industrial activities continue to increase principally because of the heavy capital outlay and maintenance of surface water development through Dams especially in developing countries (Sangodoyin and Agbawhe, 1992). Groundwater can be defined as the water that occurs beneath the surface of the earth (Larry, 1996). It is important natural resource. Many agricultural, domestic and industrial water users rely on groundwater as the sole source of low cost, high quality water.

In recent years, it has become apparent that many human activities can have negative impact on the quality and quantity of ground water. Two examples are the depletion of groundwater by excessive pumping, and its contamination by waste disposal or other activities. The contaminants can be manmade, example petroleum products, nitrates or chromium. It can also occur naturally, example arsenic and salinity. One way to access the impact of existing or proposed activities on the quality and quantity of groundwater is through the use of groundwater flow and solute transport models. Based on these, this work seeks to determine the concentration of a solute, over a particular aquifer region over a period of time.

LITERATURE REVIEW

Groundwater Modeling

A model is a representation of a system. Groundwater models are computer models of groundwater flow system, used by hydrogeologists. They are physically based mathematical models, derived from Darcy's law and the law of conservation of mass (Larry, 1996). Groundwater models help the hydrogeologist to understand the response of groundwater. It tries to understand the system more, and to predict the expected natural or artificial changes in the groundwater flow system. Groundwater model helps the hydrogeologist to predict the future behavior of an aquifer system, based on the analysis of past and present observation. Models are useful tools for decision making, in the management of a water resource system. In general, two types of methods can be used to obtain solutions to groundwater models: analytical method and numerical method.

Analytical methods typically use the structure of mathematics to arrive at a simple elegant solution. But the required derivation can be quite complex. Here, we seek to obtain a functional representation for the solution of the partial differential equation. For example, a mathematical expression that gives hydraulic head (pressure and elevation head) as a function of position and time, within the aquifer. The principal limitation of this method is that the solution can only be obtained by imposing severe restrictive assumptions about the aquifer properties and boundary conditions.

In numerical method, a discrete approximation, for the solution (computed values) of the field variables at a set of specified points, within the aquifer at a set of specified time is sought. This method is more accurate than the analytical method. Numerical method has two categories: finite difference method (FDM) and finite element method (FEM).

In this work, the finite element method of numerical analysis is used, at which the domain is completely grided (cut into a grid or mesh), then solving the flow equation for each grid, then linking together, using conservation of mass across the boundary between the grid.

Flow Processes

The groundwater flow process is either based on the physics of groundwater flow or on the pumping policy. Groundwater flow can be defined as a function of the pressure head of the total amount of water available at each end of link. Example, an aquifer may be connected to another aquifer or to a surface water through a node. If one of the nodes connected to an aquifer by groundwater link is a surface water node, the water available at the node is the storage plus its inflow. If on the other hand, there is connection of an aquifer to another aquifer, through groundwater link, then the transfer of water depends on storage volume in those aquifers. The knowledge of flow from surface water to an aquifer is important for efficient use of groundwater in a particular area.

Transport Process

The phenomenon of solute transport is quite complex. It depends on several factors like, complicated structures of aquifers, non-uniformity of flow and the interaction between solutes and matrix (Istok, 1999). The intensification of groundwater exploration and the increase in solute concentration in the aquifer due to intrusion, leaking, use of fertilizer, etc., have made solute transport wide. The purpose of a model that creates certain conditions in groundwater is to calculate the concentration of dissolved chemical species in an aquifer at any specific time. Primarily, changes in chemical concentration within an aquifer are due to four distinct processes: hydrodynamic dispersion, advective transport, fluid sources where water with different compositions mix with each other and reaction in which some amount of particular dissolved chemical species may be added to the aquifer.

Uncertainties always remain, about the properties and boundaries of the groundwater system of interest. But stochastic approaches have resulted in many significant advances in characterizing subsurface heterogeneity and dealing with uncertainty.

Parameters and Equations

In modeling groundwater flow or transport process, the following parameters are employed in the development of the mathematical equations that describe the groundwater flow process. They are: hydraulic head, storage coefficient, porosity, transmissivity and groundwater velocity. Hydraulic head refers to the elevation of a water body, above a particular datum level. Changes in the hydraulic head (H) are the driving force which causes water to flow, from one place to another. It is composed of pressure head (w) and elevation head (z). Hydraulic head is a directly measurable property. Storage coefficient is the volume of water given up per unit horizontal area of an aquifer, unit drop of the water table. Porosity indicates the amount of pore space between unconsolidated soil particles within a fractured rock. Transmissivity measures the aquifers ability to transmit water, while groundwater velocity determines the amount of groundwater, discharging through a given portion of aquifer.

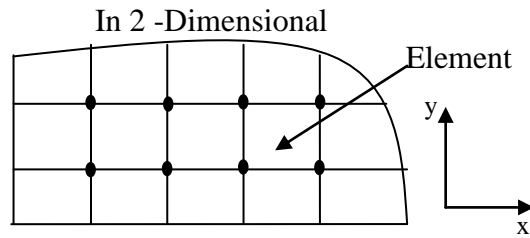
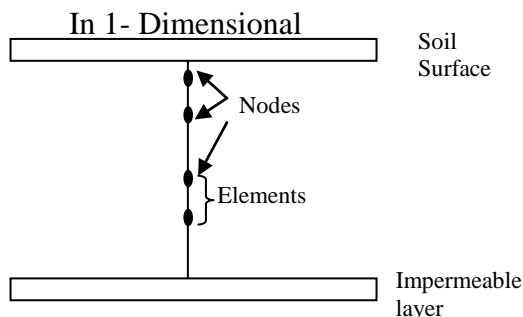
DATA ACQUISITION AND INTERPRETATION

Description of Hypothetical Site

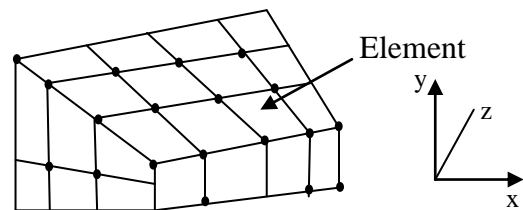
The region is a confined aquifer, composed of sand and clay. It is assumed that there is one pumping scenario applied on the same aquifer, with two observation wells located at different positions in the site. The aquifer is bounded at one side by a sea.

Data Acquisition

The first step in the solution of a solute transport problem by finite Element Method is to discretize the problem domain (aquifer). This is done by replacing the problem domain with a collection of nodes (nodal points) and elements referred to as finite element mesh.



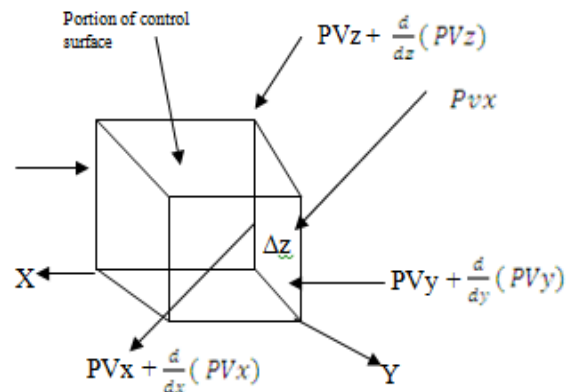
In 3- Dimensional



The size and shape of the element is determined primarily by the size and shape of the problem domain. In problems with simple geometry, fewer elements are required. The next step is to translate the conceptual model into mathematical terms. The result is a mathematical model, consisting of one or more differential equation and a set of auxiliary conditions.

Data Interpretation

Considering a unit volume of porous media (control volume):



The boundaries act as control surface. According to the law of conservation of mass,

$$\text{Net rate of inflow} = \text{inflow} - \text{outflow} = 0 \quad (1)$$

Suppose the rate at which groundwater enters the control volume per unit area is $\rho v_x, \rho v_y$ and ρv_z . The net rate of inflow in x – direction is

$$\rho v_x - \left(\rho v_x + \frac{\partial}{\partial x} (\rho v_x) \right) = -\frac{\partial}{\partial x} (\rho v_x) \quad (2)$$

i.e., law of conservation of mass, where ρ = groundwater density, v = groundwater velocity. Also the rate of inflow in y and z directions are:

$$-\frac{\partial}{\partial y} (\rho v_z) \quad (3)$$

and

$$\frac{\partial}{\partial z} (\rho v_z) \quad (4)$$

Since the rate of flow for the entire control volume is zero:

$$-\frac{\partial}{\partial x} (\rho v_x) - \frac{\partial}{\partial y} (\rho v_y) - \frac{\partial}{\partial z} (\rho v_z) = 0 \quad (5)$$

Assuming that ρ is constant (product rule):

$$-\frac{\partial}{\partial x} (\rho v_x) = \left[-\rho \frac{\partial v_x}{\partial x} + v_x \frac{\partial \rho}{\partial x} \right] = \rho \frac{\partial v_x}{\partial x} \quad (6)$$

since ρ appears outside, it cancels out,

$$-\frac{\partial v_x}{\partial x} - \frac{\partial v_y}{\partial y} - \frac{\partial v_z}{\partial z} = 0 \quad (7)$$

but according to Darcy's law,

$$\begin{aligned} v_x &= -\frac{k_x \partial h}{\partial x} \\ -v_y &= -\frac{k_y \partial h}{\partial y} \\ -v_z &= -\frac{k_z \partial h}{\partial z} \end{aligned} \quad (8)$$

Substituting into (7) we have:

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(k_z \frac{\partial h}{\partial z} \right) = 0 \quad (9)$$

for 2 - ∂ :

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial h}{\partial y} \right) = 0 \quad (10)$$

for 1 - ∂

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial h}{\partial x} \right) = 0 \quad (11)$$

where, $\partial x, \partial y$ and ∂z = components of hydraulic conductivity. ∂h = change in hydraulic head.

Derivation of Finite Element Equation

Finite element equation could be by direct method, or residual method. The method of weighed residuals would be used.

Method of Weighed Residual

Here, an approximate solution to the initial value problem is defined, and then substituted into the given equation. An error thus occurs at each point in the problem domain. We then force the weighted average of the residual for each node in the mesh to be zero.

Considering the differential equation:

$$L [\Phi(x, y, z)] - F[x, y, z] = 0 \quad (12)$$

L = differential operator

Φ = field variable

F = known function

Define an approximate solution ϕ of the form:

$$\Phi(x, y, z) = \sum_{i=1}^m N_i(x, y, z) \Phi_i \quad (13)$$

N_i = Interpretation function

Φ_i = Unknown field variable at the nodes

M = Number of nodes in the mesh.

If the approximate solution is substituted into Equation (12), the differential equation is no longer satisfied exactly, i.e.:

$$L[\Phi(x, y, z)] - F[x, y, z] R(x, y, z) \neq 0 \quad (14)$$

R = Residual error, due to the approximate solution

The residuals vary from point to point within the problem domain. Therefore we cannot force R to be zero at certain specified points because the residual may become unacceptably large, elsewhere in the domain. In method of weighed residuals, we force the weighted average of the residuals at the nodes to be zero, at each node.

$$\int_{\Omega} w(x, y, z) R(x, y, z) \partial\Omega = 0 \quad (15)$$

w(x, y, z) = weighting function, Ω = length (1 - d), area (2 - d) or volume (3 - d)

Substituting Equation (14) into (15), we have:

$$\iint_{\Omega} \int w(x, y, z) [L\Phi(x, y, z) - F(x, y, z)] \partial\Omega = 0 \quad (16)$$

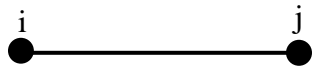
To evaluate (16), the mathematical form of the approximate solution, ϕ and the weighing function W must be specified. In finite element method, ϕ is defined in piece wise fashion, over the problem domain. The value of ϕ within any element is given by:

$$\Phi(e)(x, y, z) = \sum_{i=1}^m Ni(e)\Phi_i \quad (17)$$

Ni (e) = Element interpretation function, (i.e., one function per node).

Φ_i = Known values of field variables at each node.
m = number of nodes, within each element.

Example



An approximate solution for a one-dimensional element, within the nodes i and j can be written

$$\Phi(e)(x) = Ni(e)(x)\Phi_i + Nj(e)\Phi_j \quad (18)$$

or in a matrix form:

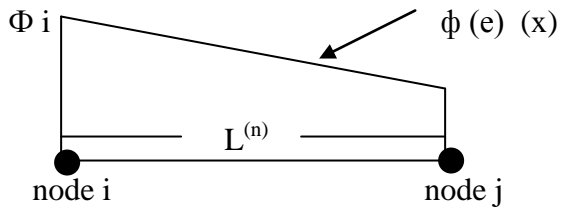
$$\Phi(e)(x) = [N(e)]\{\Phi\} \quad (19)$$

where

$$[N(e)] = [N(e)(x)Nj(e)(x)]$$

$$\{\Phi\} = \begin{Bmatrix} \Phi_i \\ \Phi_j \end{Bmatrix}$$

For the element shown below,



The interpolating function or linear function of x is:

$$Ni(e)(x) = \frac{Xj(e) - X}{L(e)} - X \quad (20)$$

$$Nj(e)(x) = \frac{X - Xj(e)}{L(e)} - X \quad (21)$$

$Xi(e)$ and $Xj(e)$ = Coordinates of the nodes
 $L(e)$ = Element length = $Xj(e) - Xi(e)$
These interpolating functions are plotted.

The value of Ni (e) is at one node i and decreases linearly to zero at node j. While the value of Nj (e) is one at node j, decreases linearly to zero at node i.

$$\phi(e)(Xj) = Ni(e)(Xj)\Phi_i + Nj(e)(Xj)\Phi_j \quad (22)$$

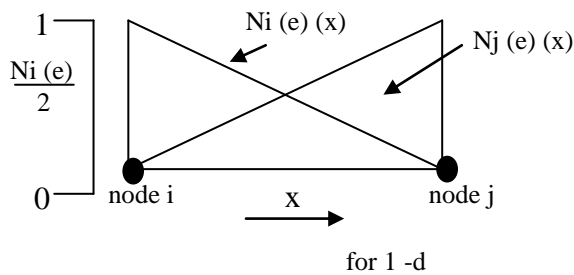
At node $j(x = Xj(e))$

$$\phi(e)(Xj) = Ni(e)(Xj)\Phi_i + Nj(e)(Xj)\Phi_j \quad (23)$$

And at midpoint of the element:

$$\left[x = \frac{Xj(e) + Xi(e)}{2} \right]$$

$$\Phi(e)(Xj) = Nj(e)(Xj)\Phi_i + Nj(e)(Xj)\Phi_j \quad \Phi(e)(x) = \frac{\Phi_i + \Phi_j}{2} \quad (24)$$



The several subsets of weighed residuals are defined by the choices of weighing functions.

- i) Subdomain method
- ii) Collocation method
- iii) Galerkins method

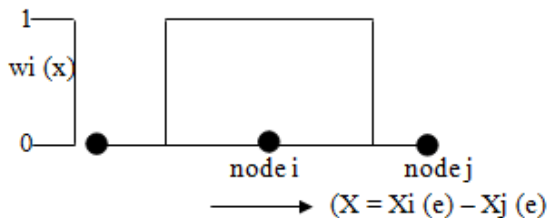
Sub-domain Method

Here, the value w is equal to one, within a small part of the problem domain. The size of the subdomain is usually chosen to be equal to the size of the element, containing the node. In 1 – dimensional cases.

$$w_i(x) \begin{cases} 1 & \text{for } (x_i = \frac{L(e)}{2}) \leq x \leq (\frac{x_i + L(e)}{2}) \\ 0 & \text{otherwise} \end{cases}$$

where,

$L(e)$ = Length of the element
 $L(e) = x_j(e) - x_i(e)$



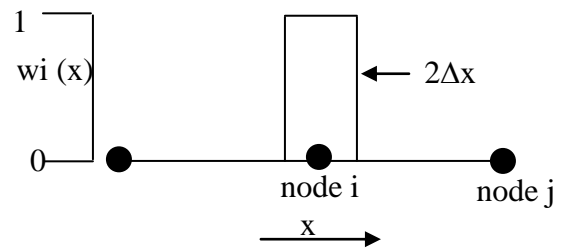
Collocation Method

A special case of the subdomain method. When the subdomain is chosen to be very small.

$$w_i(x) = \delta(x_i \pm \Delta x)$$

- δ = dirac delta function
- Δx = some small distance.

Within a distance Δx of node i
 $w_j(x) = 1$ otherwise
 $w_i(x) = 0$



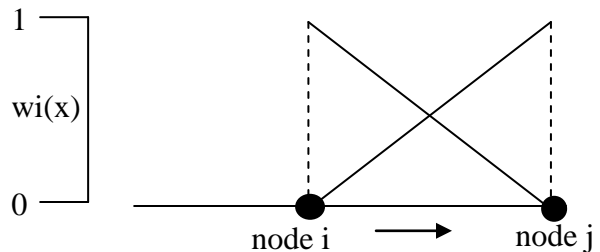
Galerkin Method

Here, the weighing function for a node is identical to the interpolation function, used to define the approximate solutions Φ . For 1 – dimensional

$$w_i(x) \frac{x_j - x}{L} \text{ for } x \geq x_i$$

$$w_i(x) \frac{x - x_i}{L} \text{ for } x < x_i$$

which is plotted as:



The Galerkins method is most commonly used to solve ground water and solute transport problems. After specifying the form of the approximate solutions and weighing functions, we can evaluate the integral in Equation (16) to obtain a system of linear equation of the form.

$$[K][\Phi] = [f] \tag{25}$$

which can be solved for the values of the field variable at each node in the mesh.

Transport Equation

- In a porous media, solute transport occurs by;
- i) Advection
 - ii) Diffusion
 - iii) Mechanical Dispersion

Advection

Here, dissolved solids are carried along with the flowing ground water. The amount of solute being transported is a function of its concentration in the ground water, and the quantity of water that is flowing. The process of advection transport process is also known as convection.

Mathematically, the one dimensional mass flux (F_L) due to advection is equal to the average linear velocity V_L (from Darcy's law), multiplied by the product of the effective porosity n_e and concentration C of the dissolved solids.

$$F_L = V_L n_e C$$

The one dimensional advection transport or the change in concentration, with respect to time dc/dt is equal to the average linear velocity, times the change in concentration with respect to a distance dc/dl . In the advection transport process, solutes are transported by the bulk motion of the flowing ground water.

Diffusion (Self Diffusion, Molecular Diffusion or Ionic Diffusion)

Diffusion occurs when a solute moves under the influence of thermal kinetic energy, in the direction of its concentration gradient. Diffusion continuous until the concentration gradient is zero.

In technical terms, the mass flux F ($\text{kg m}^{-2} \text{S}^{-1}$) of a diffusion substance passing thru a given cross-section per unit time is equal to the concentration gradient dc/dl , where C (in kg m^{-3}) represents the solution concentration and L the distance in meters, multiplied by D ($\text{m}^2 \text{S}^{-1}$) the diffusion coefficient. This relationship is known as Fick's first law. The diffusion coefficient D , for major ions (Na, K, Mg, Cl, HCO_3 and SO_4) in groundwater at 25°C varies from 1×10^{-9} to $2 \times 10^{-9} \text{m}^2 \text{S}^{-1}$. D is temperature dependent, and it is lower by about 50% at 5°C (the temperature of most groundwater than at 25°C).

In terms of the 3 components of solute transport in x,y,z directions. The net rate of solute transport by diffusion is given by:

$$F_x = -D \frac{dc}{dx}, F_y = -D \frac{dc}{dy}, F_z = -D \frac{dc}{dz}$$

The apparent diffusion coefficient D for a solute in porous media is much smaller than the diffusion coefficient for the same solute in aqueous solution do:

$$D_{\text{(porous media)}} = w(\theta) D_0_{\text{(aqueous media)}}$$

$w\theta \Rightarrow$ Empirical correction factor ie a function of volumetric water content values of w range from 0.01 for very dry soils to 0.5 for saturated soils.

The small size of apparent diffusion coefficient means that the rate of solute transport by diffusion is usually small, relative to the rate of solute transport by advection and dispersion.

Mechanical dispersion

Groundwater moves at rates that are both greater and less than the average linear velocity. This is caused by 3 effects.

- i) Differences in pore size
- ii) Tortuosity (branching and interfingering of pore channels)
- iii) Differences in the velocity of the water, across the pores, because of the drag, caused by the roughness of the pore surfaces.

Since all the water, flowing in a porous medium is not traveling in the same velocity, mixing occurs at flow paths. This mixing is called mechanical dispersion. It results in dilution of the solute at the advancing edge of the flow the mixing that occurs in the direction of the flow path is called longitudinal dispersion.

Mechanical dispersion thus refers to a mixing or spreading process, caused by small scale fluctuations in groundwater velocity, along flow path within the individual pores. On a large scale, mechanical dispersion can also be caused by the presence of heterogeneities (e.g., clay or fault) within the aquifer.

The rate of solute transport, by mechanical dispersion is given by a generalized form of Fick's law of diffusion. In terms of the 3 components of solute transport in x,y,z directions, it is given by:

$$f_x m.D = -D_{xx} \frac{\partial(\theta c)}{\partial x} - D_{xy} \frac{\partial(\theta c)}{\partial z} - D_{yx} \frac{\partial(\theta c)}{\partial x}$$

$$f_y m.D = -D_{yy} \frac{\partial(\theta c)}{\partial y} - D_{zy} \frac{\partial(\theta c)}{\partial x} - D_{yx} \frac{\partial(\theta c)}{\partial y}$$

$$f_z m.D = -D_{zz} \frac{\partial(\theta c)}{\partial z} - D_{xz} \frac{\partial(\theta c)}{\partial y} - D_{yx} \frac{\partial(\theta c)}{\partial z}$$

where,

D_{xx} , D_{yy} , $D_{zz} \Rightarrow$ coefficient of mechanical dispersion, computed from:

$$D_{ij} = a_{ij} km \frac{V_m V_n}{\sqrt{V_m^2 + V_n^2}}$$

where i and $j =$ the 3 co-ordinate directions x, y, z .
 V_m & $V_n =$ components of pore water velocity, as opposed to the apparent groundwater velocity used in Darcy's law.

M & $n \Rightarrow$ Directions of the principal components of pore water velocity. Components of pore water velocity are computed from:

$$v_x = vx\sqrt{\theta}$$

$$v_y = vy\sqrt{\theta}$$

$$v_z = vz\sqrt{\theta}$$

$\theta =$ Volumetric water content of porous media.

$a_{ijkm} \Rightarrow$ Components of aquifer dispersivity. But if the aquifer is assumed to be isotropic, with respect to dispersion all the components of the aquifer dispersivity are zero.

CONCLUSION

The use of water cannot be over emphasized, both industrially and domestically. It is established that the problem related to water is due to the contamination of the water source. To reduce the problem, the understanding of the flow pattern of the water source needs to be determined. The FEM provides a step by step solution for the solute transportation in groundwater. It provides approximate solutions as shown in foregoing discourse.

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