NATURAL TRACER TEST SIMULATION BY STOCHASTIC PARTICLE TRACKING METHOD

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ABSTRACT

Stochastic particle tracking methods are well adapted to 3D transport simulations where discretisation requirements of other methods usually cannot be satisfied. They do need a very accurate approximation of the velocity field. The described code is based on the mixed hybrid finite element method (MHFEM) to calculate the piezometric and velocity field. The random-walk method is used to simulate mass transport. The main advantages of the MHFEM over FD or FE are the simultaneous calculation of pression and velocities which are considered as unknowns, the possibility to interpolate the velocities everywhere, and the continuity of the normal component of the velocity vector from one element to another. For these reasons, the MHFEM is well adapted for particle tracking methods. After a general description of the numerical methods, the model is used to simulate the observations made during the Twin Lake Tracer Test in 1983. A good match is found between observed and simulated heads and concentrations.

INTRODUCTION

If numerical dispersion is a well known problem in mass transport in porous media simulation, adequate velocity calculations have not been studied in detail. Almost all codes calculate first the heads and then the velocities by derivating the heads. This evaluation of the flow field is not very accurate because of the approximations made on the heads due to the space discretization and the used numerical techniques. On the other hand, stochastic particle tracking methods as random-walk (RW) used to simulate contaminant transport need the derivatives of the velocities. For this purpose, classical finite difference or finite element methods may not be accurate enough to calculate the flow field, especially in the neighbourhood of singularities as wells. The mixed hybrid finite element method (MHFEM) allows the simultaneous calculation of the piezometric head and velocity field. The 3D numerical flow (MHFEM) and transport model (RW) MARCHAL is used to simulate the Twin Lake tracer test performed in 1983. Only the mass of each particle has been calibrated.

THE FLOW MODEL

The 3D movement of a non compressible homogeneous fluid in a non compressible porous media is described by the equation :

$$c\frac{\partial h}{\partial t} - \nabla(K\nabla h) = f \qquad (1)$$

where c is the specific storage of the material, h the water pressure, K the hydraulic conductivity tensor and f the source/sink term. The basic idea of the MHFEM is to calculate simultaneously the pressure and the velocity fields over the modelled domain.

This area is discretized in parallelepipedic elements, each element E having following properties (Raviart & Thomas, 1977):

(a) ∇q_E is constant over E, q_E is the velocity ;

(b) for i=1,...,6, $q.n_{i,E}$ is constant over the side A_i of E, $n_{i,E}$ being the unit exterior normal vector of the side A_i ;

(c) q_E is completely determined by the knowledge of the fluxes Q_i through each side A_i by equation :

$$q(x,y,z) = \sum_{j=1}^{6} Q_j . w_j \qquad (2)$$

where w_j are basis functions defined by :

$$\int_{A_j} w_j . n_{i,E} = \delta_{i,j} \qquad (3)$$

where $\delta_{i,j}$ is the Kronecker delta.

The mixed hybrid approximation consists in calculating simultaneously the pressure P and the velocity fields. Over each element E, we approximate the pressure by P_E, the mean pressure in E, and $TP_{E,i}$, the mean pressure on each side $A_{E,i}$. The velocity is approximated by $Q_{E,i}$, the fluxes on each side of the element E and the velocity can be calculated everywhere using equation (2). The 13 unknowns P_E, $TP_{E,i}$ and $Q_{E,i}$ must satisfy following equations :

(a) for each internal side A, we must have continuity in pressure and fluxes, that means :

$$TP_{E',i} = TP_{E,i} \quad \text{and} \quad Q_{E',i} + Q_{E,i} = 0 \qquad (4)$$

(b) P and q are related by Darcy's law :

$$q = - K \nabla P \qquad (5)$$

By writing (1) and (5) in a variational formulation using w_j defined by (3) as basis functions and taking into account continuity in pressure and fluxes between two adjacent elements, the system of equations can be solved using $TP_{E,i}$ as main unknowns (Chavent & Jaffre, 1987, Kaasschieter, 1990, Mosé et al., 1990).

Comparisons between MHFEM and finite difference (FD) have been done on a modelled domain with two prescribed head boundaries (North and South) and two impervious boundaries (East and West) and uniform permeability. A pumping well is located at 41m, 31m. Flowpaths calculated by both methods on an irregular grid are shown in figure 1a and 1b. The velocity of the moving particle describing the path is interpolated using equation (3) for the MHFEM and bilinear interpolation for the FD as given in Goode (1990). The flow paths are very similar to those obtained by the analytical solution. Even if the flow paths are well described, the travel time distribution in the neighborhood of the well is quite different from the one obtained by the analytical solution particularly near the stagnation point. Figure 2a and 2b show the relative error (travel time calculated analytically minus travel time calculated numerically over travel time calculated analytically) distribution. A quite better approximation is obtained by the MHFEM. The price to pay for that is the increase of the number of unknowns (one per side of each parallelepipedic element) over FD (one per element). More detailed comparaisons between MHFEM and FD or finite element method are given in Mosé (1990).

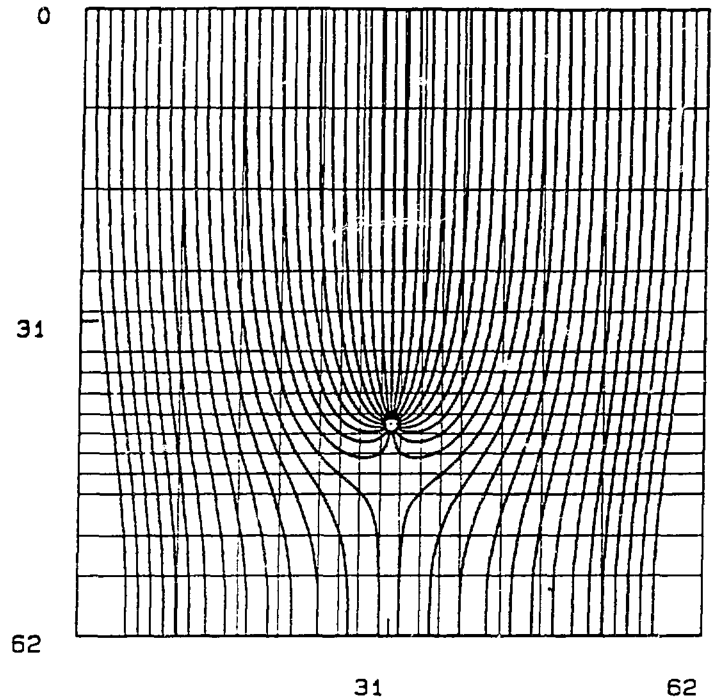
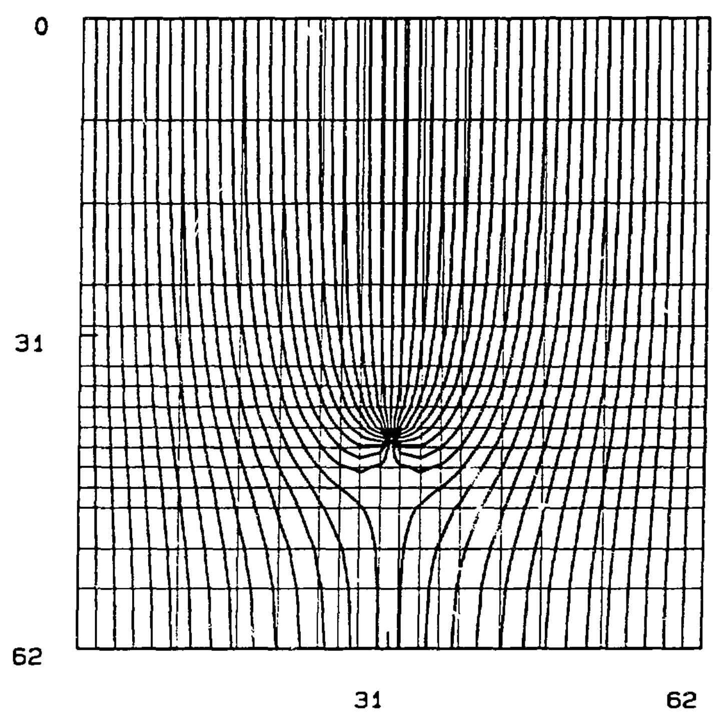


FIG. 1a : Space discretization and flow paths calculated by Finite Difference



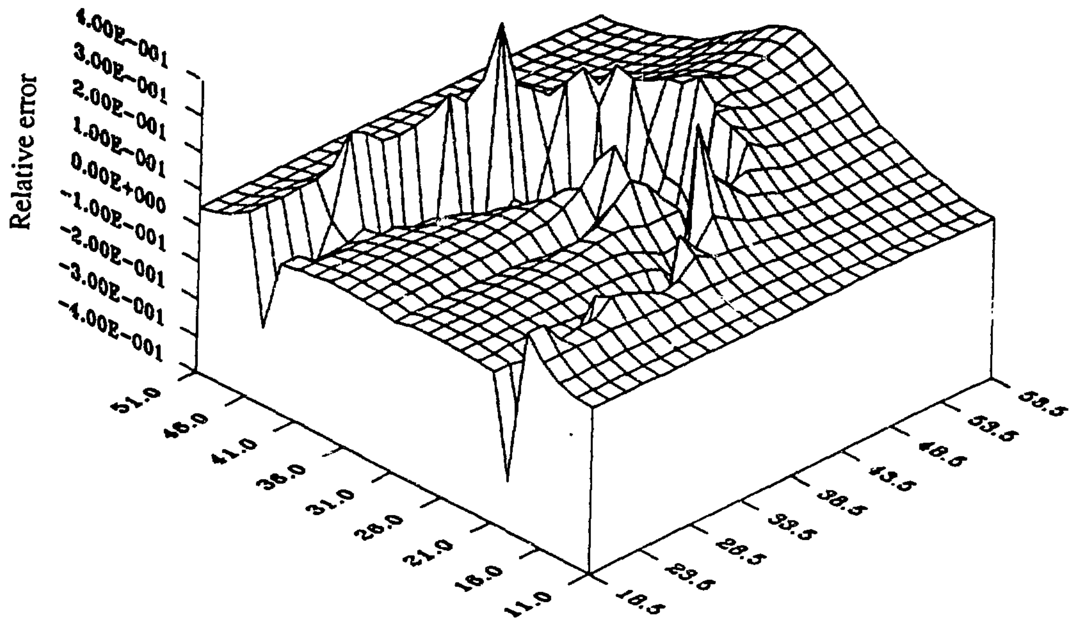


FIG 2a : Relative error in travel time distribution calculated by Finite Difference.

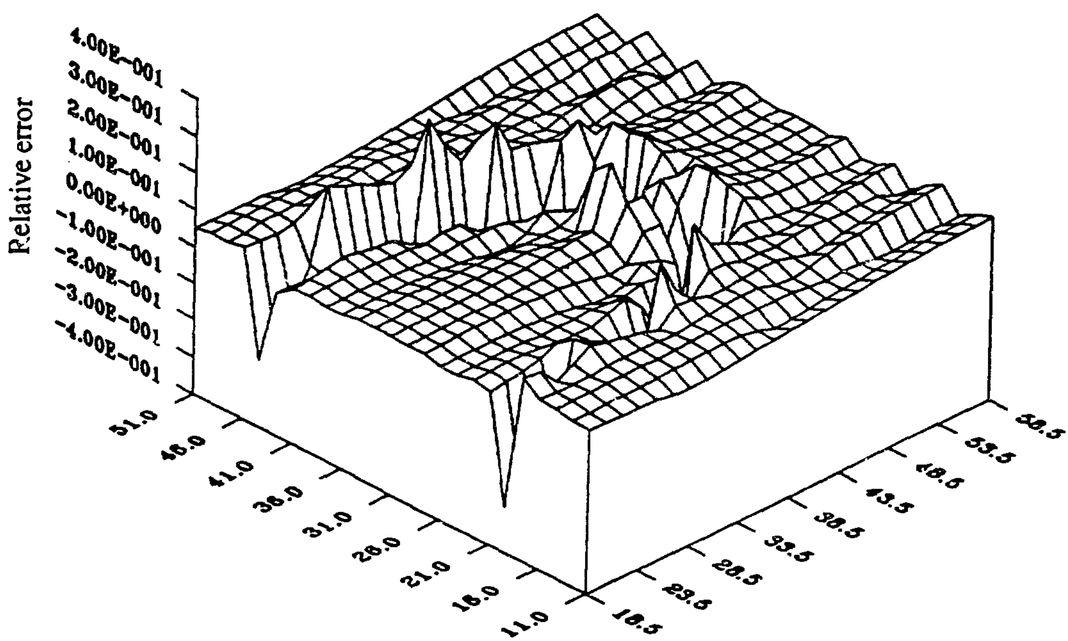


FIG 2b : Relative error in travel time distribution calculated by MHFEM.

The main advantage of this method is that the velocity field is calculated without derivating the pressure field and that the normal componant are continuous from one element to the other. In case of a heterogeneous porous medium, there is no smoothing of the velocity due to interpolation techniques as it has been shown by Goode (1990) for finite difference and there are no problems at element boundaries as it appears for finite element techniques.

THE MASS TRANSPORT MODEL

The mass transport in porous media may be described by a macroscopic driving force, advection, on which some random fluctuations are added. The random fluctuations are due to the velocity variations around the average velocity in correlation with permeability variations of the porous matrix observed at a macroscopic scale. The theory of stochastic differential equations treats these fluctuations in a certain mathematical idealization.

Let us consider a variable X which changes during time t. We choose a discrete set of times t_i with constant time step Δt. The impact of the driving force and the fluctuating forces can be described by :

$$\Delta X(t_i) = u(X(t_{i-1})) \,.\, \Delta t + Z(t_i) \qquad (6)$$

where $\Delta X(t_i) = X(t_i) - X(t_{i-1})$, u is the average velocity and $Z(t_i)$ the random fluctuations. We assume that the average of Z, $< Z(t_i) > = 0$. Otherwise, Z would contain a part which acts in a coherent fashion and could be added to the driving force.

We assume that the fluctuations at different time t_i and t_j are uncorrelated. Therefore, we may postulate :

$$< Z(t_i) \,.\, Z(t_j) > = \delta_{i,j} \, M.\Delta t \qquad (7)$$

where $\delta_{i,j}$ is the Kronecker delta at time t_i, t_j which expresses the statistical independance of Z at time t_i and t_j, and M a measure for the size of the fluctuations and equal to 2.D, D being the dispersion coefficient. In a non-uniform flow field, an important question arises concerning at which time the variable X in D must be taken (e.g. Gardiner, 1983). After Itô's definition, $D = D(X(t_{i-1}))$ that means that D at time t_i and $X(t_{i-1})$ are uncorrelated. On the other hand, Stratonovitch's definition gives $D = D(X([t_i + t_{i-1}]/2))$ which is more close to the reality, fluctuations go on all the time. The Stratonovitch scheme is difficult to compute, so that the Ito scheme is quite widely used. The stochastic differential equation is then the following :

$$X(t_i) = X(t_{i-1}) + u(X(t_{i-1}))\Delta t + z\sqrt{2\,D(X(t_{i-1}))\Delta t} \qquad (8)$$

It has been shown that this equation is equivalent to the Fokker-Planck equation (e.g. Gardiner, 1983) :

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial X_i}(uf) + \frac{\partial^2}{\partial X_i \partial X_j}(Df) \qquad i=1,2,3 \quad j=1,2,3 \qquad (9)$$

To be equivalent to the transport equation, a term has to be added to the driving force (Ackerer & Kinzelbach, 1985 ; Ackerer 19987 ; Uffink 1987, 1990). For a coordinate system with its x axis parallel to the velocity, the equivalent stochastic differential equations to the 3D convection-dispersion equation are the following :

$$x(t_i) = x(t_{i-1}) + \left[u(x(t_{i-1})) + \frac{\partial D_L(x(t_{i-1}))}{\partial x} \right] \Delta t + z_1\sqrt{2D_L(x(t_{i-1}))\Delta t}$$
$$y(t_i) = y(t_{i-1}) + \frac{\partial D_T(y(t_{i-1}))}{\partial y} \Delta t + z_2\sqrt{2D_T(y(t_{i-1}))\Delta t} \qquad (10)$$
$$z(t_i) = z(t_{i-1}) + \frac{\partial D_T(z(t_{i-1}))}{\partial z} \Delta t + z_3\sqrt{2D_T(z(t_{i-1}))\Delta t}$$

where x,y,z are the coordinates of the particle at time t_i, u the average pore velocity, D_L and D_T the longitudinal and transverse dispersion coefficients, Δt the time step and z_1, z_2, z_3 random numbers with a normal distribution with 0 mean and standard deviation equal to 1.
The simulation consists in injecting many particles and make them jump following equations (10). Concentrations are calculated by counting particles in a volume, each particle having a given mass related to the number of injected particles and the mass flux of the pollutant source.
The main advantage of this method is that it is free of numerical dispersion, mass conservative and the two moments of the particle distribution (i. e. the mean velocity and the apparent dispersion of the tracer cloud) are very easy to calculate. For solute transport in 3D, it is often the way of last resort at large scale (Kinzelbach, 1987). This method is very nice to compute. It does not require area discretization and there is no system of equations to solve i.e. you do not need computer with large memory. Stochastic particle tracking techniques show fluctuations in concentration due to the random process. It is possible to smooth the results by increasing the number of particles. The fluctuations are proportional to the square root of the number of particles in a given volume so that increasing the number of particles does not bring a proportional improvement in the precision of the results. Therefore, at reasonable computational effort, parameter sensitivity cannot be performed for low sensitive parameters.
The same presentation of the flow and transport model is also given in Ackerer et al. (1990).

SIMULATION OF THE TWIN LAKE TRACER TEST

Detailed descriptions of the the Twin Lake Tracer tests are given in e.g. Killey and Moltyaner (1988).The location of the piezometers, multilevel samplers and dry access tube, the piezometric head distribution and the evolution of concentration in space and time come from the Twin Lakes Database.
In order to have detailed head boundaries for the flow model, the modelled area has been limited at 5m from the injection well to 30m from the injection well. This limitation is due to the insufficent head values around the injection well available in the database. The grid has also been rotated so that its main axis is parallel to the axis of flow given in Killey and Moltyaner (1988). The modelled area is a parallelepiped of 25 m in the length, 8m in the width and 9,50m in the height. The lower left corner of the grid is located at 30m west and 8m south from the injection well and at 142,0 m depth. Each element of the grid has following dimensions : Δx =1m, Δy=1m, Δz=0,5m. The hydraulic conductivity distribution used in the model is the one given in Killey and Moltyaner. The head is prescribed at the west and east boundaries the north and south boundaries are supposed to be zero flux boundaries. No calibration has been performed to simulate the head. The average of the absolute values in head differences between measurement and simulation is equal to 4,6 cm and the standard deviation to 4,3 cm for 197 measurement points.
15000 particles have been used to simulate the tracer transport. Longitudinal and transverse dispersivity coefficients used for the simulation are mean values of dispersivities calculated by Moltyaner and Killey (1988a, 1988b), i.e. α_L = 6cm, α_T=0,1cm. Upstream boundary conditions are the measured concentrations over time and space at 5m from the injection well. This boundary may be more accurate than the concentration in the well because of its unknown distribution in space around the well. The travel time from the injection well to the boundary is supposed to be equal to 2.5 days. Figure 3 shows the comparison between measured (solid line)

and simulated (dashed line) concentrations along the axis of flow going through the injection well. A good match between measurement and simulation is also achieved on each part of this flow axis (Fig. 4). The differences in the peak arrival time at depth 145,0m is constant over the path line. It is not due to permeability variations which are not taken into account but probably to a different peak arrival time at the upstream boundary which varies from 1,83 to 4,08 days (Killey and Moltyaner, 1988). Some important discrepancy appears at the tracer plume boundary. To perform this simulation, the mass of each particle was the only fitted parameter.

CONCLUSIONS

In groundwater transport contamination modelling, special care has to be given on the flow field calculation. MHFEM is an accurate numerical method for flow field calculation. Even if flow paths are well described, errors in velocity magnitude can be underlined by travel time computations.

With accurate numerical techniques, 3D flow and transport simulation are feasible without having recourse to supercomputers. The simulation of the Twin Lake tracer test were made on 386 PC / 25 MHz and on a supercomputer IBM 390/VF. The whole simulation (flow and transport) needs about 5 hours computation time on the PC in extended mode and 4 minutes on the IBM. The total number of unknowns is equal to 12227 and the number of injected particles equal to 15000. The mass transport were performed in 35 time steps.

The accurate data interpretation of the Twin Lake tracer test (1983) leads to sufficient information over the hydraulic conductivity distribution, the ratio between vertical and horizontal permeability, the longitudinal and transverse dispersivity and the porosity to perform satisfactory simulation. However, more informations about the validity of the data set and the model may be given by the simulations of the tests made in 1982 and 1987.

The Twin Lake aquifer may be defined as a more or less homogeneous aquifer with some well defined layers of finite length. In more heterogeneous porous media, the space discretization has to be adapted to the size of the heterogeneity in order to perform a accurate simulation of the flow field. The magnitude of the dispersivity used in simulations is related to the space discretization and to the knowledge of the permeability distribution."Numerical tracer tests" made with very accurate numerical models may be considered as a usefull tool to improve our understanding in space discretization related to spatial variability of the hydraulic conductivity and porosity.Although the spatial variability of porosity is less than the variability of permeability, it may be taken into account because of its important rule in lateral mixing between layers.

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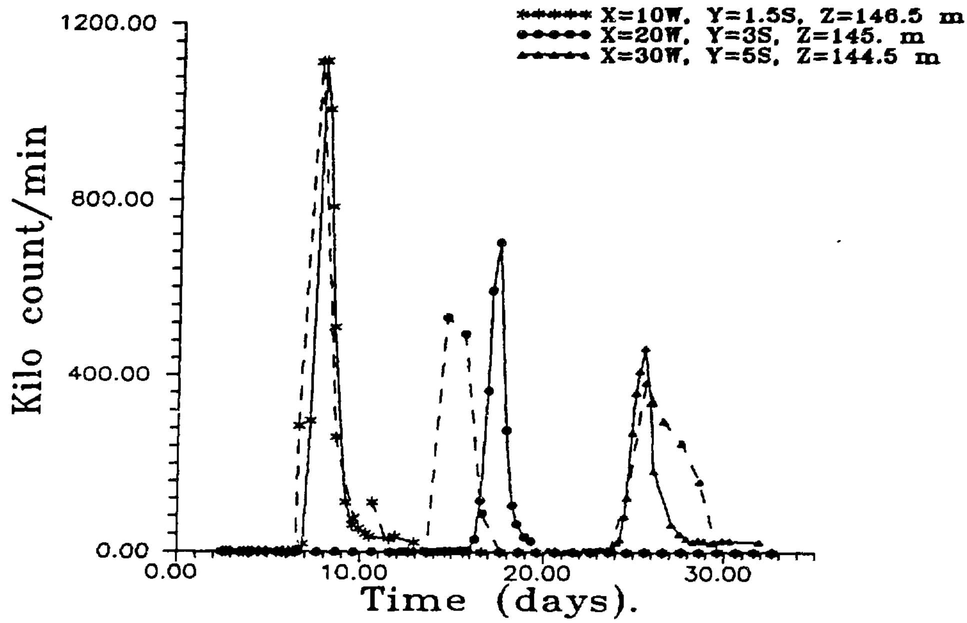


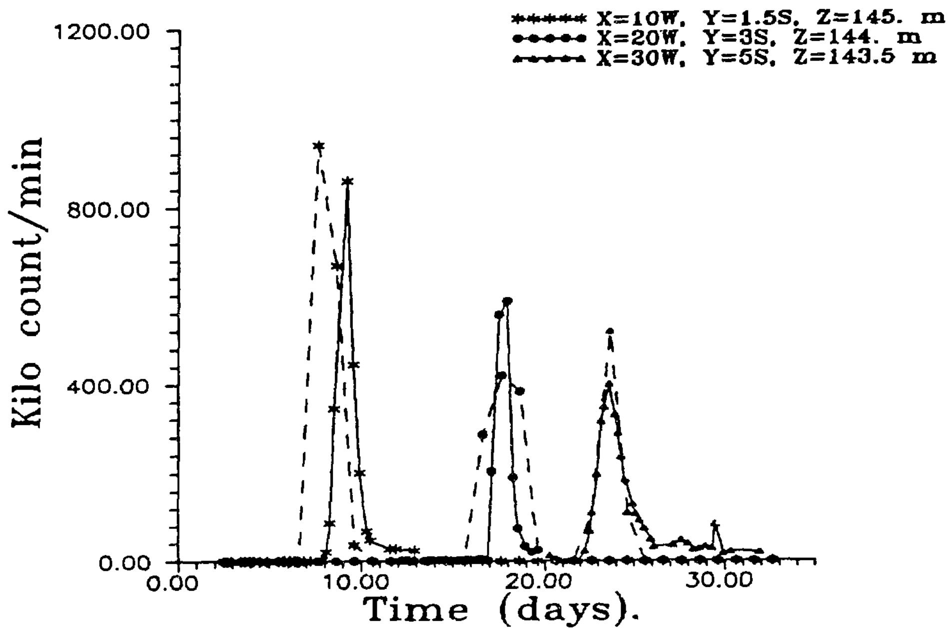
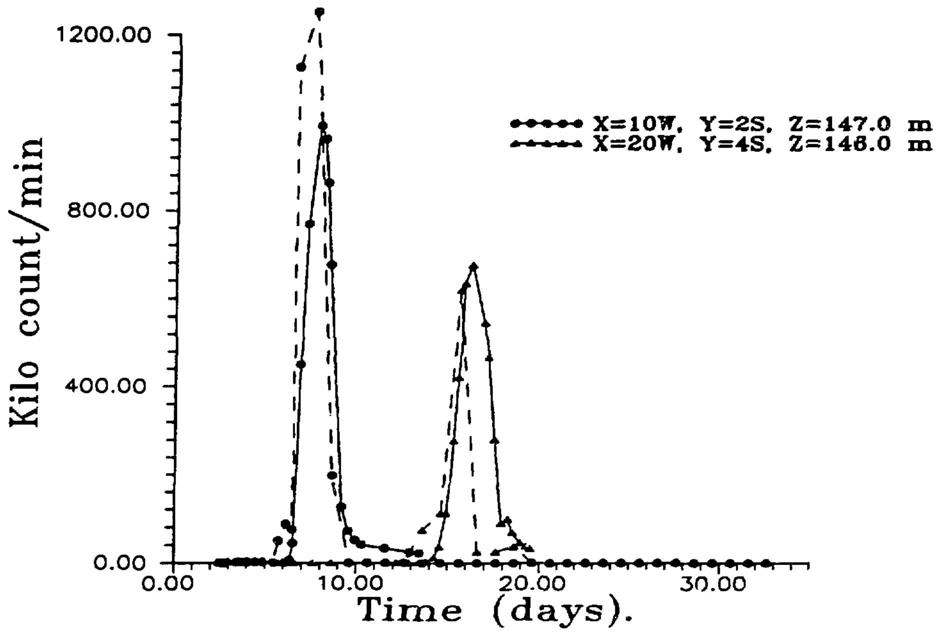


FIG 3 : Comparisons between measured (solid line) and simulated (dashed line) concentrations along the axis of flow going through the injection well.



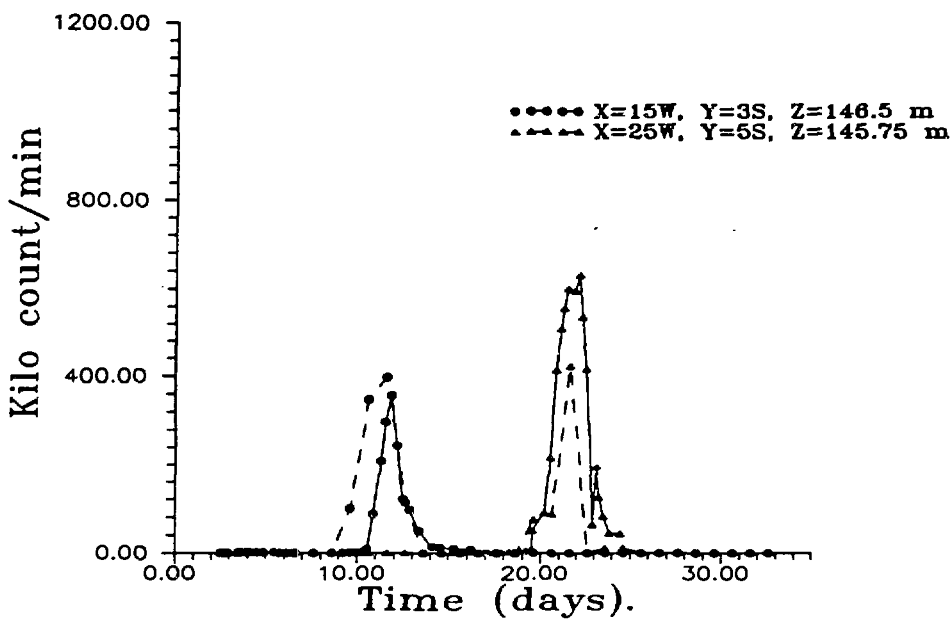


FIG 4 : Comparisons between measured (solid line) and simulated (dashed line) concentrations on each part of the axis of flow going through the injection well.

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