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ANALYSIS AND NUMERICAL SIMULATION OF SINGLE-WELL TRACER TEST IN HOMOGENEOUS, LAYERED AND SLIGHTLY TILTED FORMATIONS

تحليل و محاكاة عدديه لاختبار حركه المذيب المحقون من بئر فردى في تكوينات

متجانسه وطبقيه ومائله بميل خفيف

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فى هذا البحث تم عمل تحليل ومحاكاة عديه لاختبار حركه المذيب من بئر حقن فردى فى حقل سريان متماثل حول المحور الرأسى لطبقه حامله للمياه ذات خصائص حيدر وليكيه متجانسه وأخرى طبقية وأخرى مائله بميل خفيف . وقد تم التحقق من المحاكه العددية من خلال النموذج الرياضى التحليلى المشتق فى هذه الدراسه ، لقد أثبتت النتائج توافق ممتاز بين النموذج التحليلى و المحاكه العدديه فى حالة التكوين ذو الطبقات الافقية . ركزت الدراسه أيضا على الاختلاف بين ميكانيكيات النقل فى حالة السريان القطرى و المريان الموحد أظهرت النتائج أن متوسط الجذر التربيعى لنفاذيه الطبقات هو الممثل الفعال للوسط فى حاله السريان القطرى بالحمل فى تكوين طبقى.

ABSTRACT

Simulation of a field tracer experiment from an injection well in an axially symmetrical flow field in homogenous, stratified and slightly tilted aquifers is presented. The simulation has been verified by analytical solutions of the evolution of the first and second radial spatial moments of the tracer displacements derived in the current study under pure advective transport in case of layered formation. The study focused also on the discrepancies in the transport mechanisms between uniform (linear) and axially symmetrical radial flow fields in homogenous, layered and slightly tilted formations. Excellent agreement exists between analytical solution and the numerical simulation for the case of pure advection in both first and second moments supporting the validity of the numerical simulations. A subdiffusive dispersion regime in case of transport by advection and dispersion in homogenous aquifer is observed due to the decline of the velocity field. $\langle \sqrt{K_n} \rangle$ is the representative effective medium of the layered aquifer in case of pure advection under axially symmetrical flow field.

1. INTRODUCTION

Field tracer experiments are mainly used either to evaluate hydraulic parameters (e.g. hydraulic conductivity, transmissivity, porosity, storage coefficient, etc.), dispersive parameters (e.g. dispersivities, dispersion coefficients, retardation factor, etc.) of aquifers or to validate flow and transport models. Many researchers have developed mathematical

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C. 14

methods to interpret and analyse field experimental results. Some recent studies e.g. Swamce, P. K. and Ojha, C. S. [1990], among may others, concerned with pumping test analysis to evaluate hydraulic parameters of confined and leaky aquifers. They focused on the unsteady groundwater flow in homogeneous isotropic aquifers. The work presented an empirical equation for the well function that facilitates determination of aquifer parameters. The aquifer parameters, inferred from the pumping test, are averaged over the whole aquifer within the domain of influence of the well. This type of pumping tests will be beyond the scope of the current research.

For determination of the dispersive parameters of aquifers one of the following field tests is often conducted: (1) natural gradient experiments, (2) single-well tracer experiments, and two-well tracer experiments. In this work, a focus is made on the single-well tracer experiment. However, for the sake of completeness some review is presented. Moltyaner, et al. [1993] performed a numerical simulation of Twin Lake natural-gradient tracer test. The primary objectives of the simulation were to study the influence of geological heterogeneities, field scale dispersion and to provide data for developing and evaluating groundwater flow and transport models. It was concluded that the advective-dispersive models of the local-scale transport perform better in predicting the tracer migration at the Twin Lake aquifer using measured velocities rather than velocities simulated by a flow model.

Guven, O. et al [1985] dealt with the dispersive properties of stratified aquifers based on single-well field tracer experiment. In this test, tracer is pumped into the formation for a period of time and then pumped out. Concentration data are obtained from the injection-withdrawal well and from one or more observation wells. The study was particularly to simulate the field experiment by Pickens and Grisak [1981a]. They concluded their results based on an idealized model where the flow is nearly horizontal. In designing a tracer test it is important to have some idea of the type of nonhomogeneity in the site of the test. Huyakom, P. S. et al [1986] have conducted a simulation study of two-well injection-withdrawal tracer tests in stratified granular aquifers at two sites using a finite element model (FEM). The first site is located near the Chalk River Nuclear Laboratories in Canada, and the second site is located in Mobile, Alabama. The paper focused on the field application of the proposed FEM. The model accounts for stratification in hydraulic conductivity but assumes areal homogeneity. One of the important conclusions in the paper is that stratification shows interesting effects on the spatial distribution of the concentration and on the evolution and spreading pattern of the tracer plumes. These effects have not been fully assessed in the field measurement and should be investigated further. Molz, F. J. et al (1986) reported a second type of two-well tracer test using a bromide tracer at the Mobile site. They used a quasi-three-dimensional advective model with zero hydrodynamic dispersion to simulate the test. Such flow systems result in plumes with high concentrations of contaminant moving over large horizontal distances in the higher-permeable zones. Jim Yeh, T.-C. et al [1995] have performed three-dimensional two-well forced-gradient tracer experiment of chloride plumes in a coastal sandy aquifer at Georgetwon, South Caroline. The purpose of this field experiment was to assess the ability to predict solute transport in the aquifers with extensive hydraulie conductivity data. They showed that our predictability is limited only to the bulk plume behaviour that is controlled by some significant heterogeneities.

In this paper a focus is rather made on the study of transport regimes in case of single-well tracer experiment. The study focused also on the discrepancies in the transport mechanisms between uniform (linear) and axially symmetrical radial flow fields in homogenous, layered and slightly tilted formations.

2. DERIVATION OF ANALYTICAL SOLUTION OF ADVECTIVE TRANSPORT IN LAYERED FORMATIONS UNDER AXIALLY SYMMETRICAL FLOW FIELD

The governing equation of steady axially symmetrical radial flow in non-homogeneous and anisotropic confined aquifer is given by (see Rushton and Redshaw [1979]),

$$\frac{K_r}{r} \left(\frac{\partial \phi}{\partial r}\right) + \frac{\partial}{\partial r} \left(K_r \frac{\partial \phi}{\partial r}\right) + \frac{\partial}{\partial Z} \left(K_s \frac{\partial \phi}{\partial Z}\right) = 0....(1)$$

Where r is the radial distance from the well centre [L], φ is the groundwater head [L], K_r , and K_r are hydraulic conductivities in the radial and vertical directions respectively[LT⁻¹].

By the logarithmic transform a = ln(r), Eq. 1 can be simplyfied to read,

$$\frac{\partial}{\partial a}\left(K,\frac{\partial\phi}{\partial a}\right)+r^{2}\frac{\partial}{\partial Z}\left(K,\frac{\partial\phi}{\partial Z}\right)=0.$$
(2)

In case of isotropic layered formation, the hydraulic conductivity is a function of the vertical direction, Z, so Eq. 2 can be written as,

$$\frac{\partial}{\partial a} \left(K(Z) \frac{\partial \phi}{\partial a} \right) + r^2 \frac{\partial}{\partial Z} \left(K(Z) \frac{\partial \phi}{\partial Z} \right) = 0....(3)$$

The analytical solution of Eq. 3 in case of a single fully penetrated injection well in the centre of a multi-layer aquifer as shown in Figure 1 is given by (no change of ϕ in the Z-direction and flow is horizontal),

Where Q is the well discharge $[L^{3}T^{1}]$, r_{w} is the well radius [L], and ϕ_{w} is the head at the injection well [L].

The total well discharge in multi-layer aquifer is given by.

$$Q = \frac{2\pi \left(\sum_{i=1}^{n} B_{i} K_{i}\right)}{\log_{c} \left(\frac{R}{r_{w}}\right)} (\phi_{w} - \phi_{c})....(5)$$

Where ϕ_e is the groundwater at the outer edge of the circular aquifer [L], **R** is the radius of the aquifer [L], B_i is the head thickness of layer number *i* [L], and *K*, is hydraulic conductivity of layer number *i* [LT⁻¹].



Figure 1. Definition sketch of injection well in confined aquifer with a tracer front in multi-layer aquifer.

The discharge passing through each layer is calculated by,

$$Q_{r} = \frac{2\pi(\phi_{u} - \phi_{c})}{\log_{c} \begin{pmatrix} R \\ r_{u} \end{pmatrix}} B_{r} K_{r}$$
(6)

The corresponding velocity at each layer is calculated by,

$$v_{r}(r) = \frac{Q_{r}}{2\pi r B_{r} \varepsilon} = \frac{(\phi_{w} - \phi_{\varepsilon})}{\varepsilon \log_{\varepsilon} \left(\frac{R}{r_{w}}\right)} \left[\frac{K_{r}}{r}\right].$$
(7)

Where ε is the effective porosity, which is assumed constant for all layers.

In case of slug injection of a tracer from the well along the aquifer depth under steady state groundwater flow, the displacement of the tracer front at each layer is calculated by,

$$\frac{dr_{i}(t)}{dt} = v_{i}(r) = \frac{(\phi_{u} - \phi_{c})}{\varepsilon \log_{c} \left(\frac{R}{r_{v}}\right)} \left[\frac{K_{i}}{r_{i}}\right].$$
(8)

C. 18

By separation of variables and integration one could obtain the radial displacement of the tracer front, $r_i(t)$, in layer *i* as,

$$\mathbf{r}_{i}(t) = \sqrt{\frac{\mathbf{r}_{w}^{2} + 2\frac{(\phi_{w} - \phi_{e})}{\varepsilon \log_{e} \left(\frac{R}{r_{w}}\right)}} [K_{i}] t}....(9)$$

In order to simplify calculation of spatial average of the displacements over *n* layers, assume $r_w=0$ so, the spatial average is given by.

$$\left\langle r_{i}(t)\right\rangle = \sqrt{2\frac{\left(\phi_{w}-\phi_{r}\right)}{\varepsilon\log_{r}\left(\frac{R}{r_{w}}\right)}} \left\langle \sqrt{K_{i}}\right\rangle \sqrt{t} \dots (10)$$

Where the angle brackets, $\langle . \rangle$, means the spatial average, $\langle r_i(t) \rangle$ is the spatial average displacement of the tracer front [L], $\langle \sqrt{K_i} \rangle$ is the average of square root of hydraulic conductivity over the *n* layers.

Eq. 10 shows that the mean radial displacement evolves with the square root of travel time.

The variance of the displacements around their mean, $\sigma_r^2(t)$, $[L^2]$ is given by,

$$\sigma_r^2(t) = \left\langle r_i^2(t) \right\rangle - \left\langle r_i(t) \right\rangle^2 = 2 \frac{(\phi_n - \phi_r)}{\varepsilon \log_r \left(\frac{R}{r_n}\right)} \left[\left\langle K_i \right\rangle - \left\langle \sqrt{K_i} \right\rangle^2 \right] t \qquad (11)$$

From Scheidegger [1954] and Dagan [1987], it is noted that the macro-dispersion coefficient, $D_r(t)$, is calculated as half the derivative of the variance of the displacements around its radial mean that leads to the following expression,

$$D_{r}(t) = \frac{1}{2} \frac{d\sigma_{r}^{2}(t)}{dt} = \frac{(\phi_{u} - \phi_{r})}{\varepsilon \log_{\epsilon} \left(\frac{R}{r_{w}}\right)} \left[\langle K_{r} \rangle - \langle \sqrt{K_{r}} \rangle^{2} \right].$$
(12)

The radial macro-dispersion coefficient is constant which shows Fickian regime. However, in case of uniform flow with linear hydraulic gradient, the following relations hold for the same variables mentioned above [Mereado, 1967]. The average displacement is expressed as,

Where $\langle X(t) \rangle$ is the spatial average displacement of the tracer front [L] and J_x is the linear gradient acting on the flow domain from left to right [L/L].

The variance of the displacement front is calculated by.

The longitudinal macro-dispersion coefficient is given by,

$$D_{c}(t) = \sigma_{K}^{2} \frac{J_{v}^{2}}{\varepsilon^{2}} t \qquad (15)$$

The macro-dispersion coefficient is linear in time showing a superdiffusive regime [see Sahimi 1993].

3. TRANSPORT BY ADVECTION AND DISPERSION IN AXIALLY SYMMETERICAL FLOW FIELD

In the pervious section, a focus is made to the advection transport in an axially symmetrical flow field where analytical solutions for the first and second moments of the front displacement are developed. In this section the transport model by advection and dispersion in axially symmetrical flow field is addressed. The transport equation describes the transport of dissolved substance by advection and dispersion that introduced at an injection well in an axially symmetric flow field is given by [Ogata, 1970],

$$\frac{\partial C}{\partial t} + v_r \frac{\partial C}{\partial r} - \frac{1}{r} \frac{\partial}{\partial r} \left(r D_r \frac{\partial C}{\partial r} \right) - \frac{\partial}{\partial Z} \left(D_z \frac{\partial C}{\partial Z} \right) = 0.$$
(16)

Where r is the radial co-ordinate, C = C(r, Z, t) is the tracer concentration [ML³], D_r and D_c are the radial and vertical hydrodynamic dispersion coefficients respectively [L²T⁻¹] and $v_r = v_r(r, Z)$ is the radial seepage velocity which is obtained by Eq. 7 [LT⁻¹].

The hydrodynamic dispersion eoefficients can be written as [Bear, 1979],

 $D_{r} = D_{s} + \alpha_{r} |v_{r}|$ $D_{z} = D_{s} + \alpha_{z} |v_{r}|$ (17)

Where, α_r and α_z are the radial and vertical local dispersivities [L] and D_o is the molecular diffusion coefficient which is too small and can be neglected in the current study $[L^2T^1]$.

The initial and boundary conditions of a single well tracer experiment in layered formation under a pulse injection of initial concentration C_o are,

 $C(r_{\sigma}, Z, 0) = C_{\sigma}$ C(r, Z, 0) = 0 $C(\infty, Z, t) = 0$ $\frac{\partial}{\partial Z}C(r, 0, t) = 0$ $\frac{\partial}{\partial Z}C(r, -H, t) = 0$ (18)

Where *H* is the aquifer thickness.

Analytical solutions in this case are given, in terms of breakthrough curves for continuous tracer injection, by Guven, O. et al [1985]. However, according to the author knowledge, there is no analytical solution in terms of plume spatial moments. In this paper we will resort to numerical solutions by particle tracking technique for the plume spatial moments to study the transport mechanisms in this type of flow.

4. NUMERICAL SIMULATION OF THE SINGLE-WELL TRACER TEST BY PARTICLE MODEL

To study and validate the analytical model derived in section 2, a set of numerical simulations has been performed. A hypothetical single-well tracer test in a vertical section is performed in a confined aquifer with a full penetration well of radius $r_w=0.25$ m. The aquifer consists of two layers (n=2) as shown in Figure 2 (left-top image) with a hydraulic eonductivity contrast of 10 m/day for the high permeable layer (appears in white) and 1 m/day for the low permeable layer (appears in black). The effective porosity of the aquifer is assumed to be $\varepsilon=0.35$. The aquifer extends at R=200m in radius around the well. The total aquifer depth is H=20m. The hydraulic head at the well is assumed to be $\varphi = 1$ m. The total well discharge according to this situation is 86.9 m³/day. The weighted average hydraulic conductivity of the two layers is 4.86 m/day and the corresponding average transmesivity is 102 m²/day. The aquifer hydraulic head distribution is calculated from Eq. 4. Figure 2 (second row) shows the distribution of the piezometric head field. It is of logarithmic type which means that the gradient is high near the well while it decreases far from the well.

A particle tracking random walk [Uffink, 1990] was used to solve the advectiondispersion equation with the aforementioned initial and boundary conditions (Equation 19). The numerical values for the transport model are given in Table 1. The physical parameters used in the simulations are realistic field values that are in the same order of magnitude of the two-well tracer test at the Mobile site [Molz. F. J. et al, 1986]. When a steady state groundwater flow from the injection well is reached, a mass of 1000 grams of a tracer is injected from the well into the aquifer.

C. 21 Amro M. M. Elfeki

Parameter	Numerical Value
Injected tracer mass	1000 Grams
Number of particles	5000 Particles
Time step in calculations	0.124 Day
Longitudinal pore-scale dispersivity	0.10 m
Transverse pore-scale dispersivity	0.05 m
Total aquifer thickness	20 m
X-coordinate of an observation well	100 m
Molecular diffusion coefficient	0.0

Table 1. Numerical values used in the simulation of the single-well tracer experiments.

This mass is represented by 5000 particles which are placed at the well screen over the full depth of the aquifer (i.e. at $r_w=0.25$ m and H=20m). The evolution of the particle spatial moments is monitored each time step and some snapshots of the plume at different time steps are also reported by the programme.

5. ANALYSIS OF RESULTS

The results of the simulation in terms of snapshots of the plume and the spatial moments of the particle clouds are shown in this section. Two selected snapshots of the plume at 62 and 3721 days are presented in Figure 2 for the two-layered and the corresponding homogeneized aquifer with and without the effect of pore-scale dispersion process. The results of the groundwater heads are also plotted in the same graph for both cases that are identical and show logarithmic distribution of the heads due to the effect of radial flow (second row of Figure 2). The results of the plumes show that the concentration distribution in case of introducing pore-scale dispersion process is symmetrical around the front displacement that is due to pure advection.

The spatial moment analysis provides a criterion to evaluation the performance of the analytical model. Figure 3 (top) shows the evolution of the first moment of the particle cloud (radial centroid displacement) with respect to the travel time. Excellent agreement exists between the analytical solution (solid line) and the numerical simulation (black circles). The result of the first moment shows, qualitatively, the same trend as observed in the recent field study by Tim Yeh et al [1995] (displayed in Figure 11B in their paper). The Figure displays the differences between the advective transport under axially symmetrical radial flow and uniform linear gradient flow field. The certroid is moving at a faster rate in the first ease especially close to the well this is due to the high velocity near the well. However, at a certain distance far from the well (corresponding to about 800 days) the centroid is moving slower than the case of uniform flow. The evolution of the displacement is proportional to square root of travel time in radial flow field (Eq. 10) while it is proportional to travel time in case of uniform flow (Eq. 13).



Figure 2. Simulation results in terms of piezometric head distribution and plume snapshots at two different times 62 days and 3721 days since release: (left column is the simulation of a two-layered system with and without pore-scale dispersion process, right column is the simulation of a homogeneized system with and without pore-scale dispersion process).

The centroid movement using an advection-dispersion model in a layered aquifer is slightly faster than the case of pure advection in the same layered aquifer. This is due to the dispersion coefficient at the pore scale that is dependent on the radius from the well. The dispersion coefficients D_{ri} and D_{ri} at the pore scale for layer *i* can be expressed as (substitution of Eq. 7 into Eq. 17),

$$D_{r} = D_{r} + \alpha_{r} \left| \frac{Q_{r}}{2\pi B_{r} \varepsilon} \right| \frac{1}{r} \right|$$

$$D_{r} = D_{o} + \alpha_{z} \left| \frac{Q_{r}}{2\pi B_{r} \varepsilon} \right| \frac{1}{r} \right|$$
(19)

Eq. 19 shows that the dispersion coefficient at the pore seale is inversely proportion to the radial distance from the well. Therefore, the radial dispersiou will produce random displacements that are longer near the well in comparison with the random displacements far from the well. These displacements will contribute to the advective displacements eausing faster plumes with respect to the ones undergo pure advection process. The pure advection in the homogenized aquifer (dashed lines with triangles) produce displacements that move at a faster rate in comparison with the layered model. This means the arithmetic average conductivity is not a good representation of the

C. 23 Amro M. M. Elfeki

layered medium. However, the average of square root of hydraulic conductivity over the n layers, $\langle \hat{v} K_t \rangle$ is the representative effective medium of the layered aquifer under radial flow.



Figure 3. Plume spatial moments in different cases: top is the first moment and bottom is the second moment (the five cases considered are: single-well numerical simulation with advection in two-layers, single-well analytical solution under advection, single-well numerical simulation under advection and dispersion in two-layers, single-well numerical simulation under advection and exercise and the second second

Figure 3 (bottom) shows the evolution of the second moment of the particle cloud (variance of the radial displacements around their mean) with respect to the travel time. Similar to the first moment, excellent agreement is found between the analytical solution (solid line) represented by Eq.11 and the corresponding numerical simulation (black circles). The growth of the radial variance is linear in time in case of radial flow field (diffusive regime) when compared with the case of uniform flow with linear gradient where the growth is parabolic in time (solid line with squares) showing superdiffusive regime. It is obvious that there is no growth in the variance in case of pure advection in homogenized medium (dashed lines with triangles). For completeness of the numerical experiments a simulation with advection and dispersion processes in a homogenized aquifer is performed to study the dispersion mechanism in this case. Figure 4 shows the evolution of the second moment of the particle displacements in time. The growth of the variance of the displacements displays a subdiffusive regime.



Figure 4. Radial variance of the particle displacements around their mean in case of homogenized aquifer under advection and dispersion processes.

A numerical experiment with a slightly tilted layered aquifer is also addressed (Figure 5 top image). In this experiment a pure advective model is used. The flow field is calculated numerically using finite difference scheme of the differential equation, Eq. 2, for the axially symmetrical flow field and the steady groundwater flow under uniform flow conditions in heterogeneous medium. The flow field in both eases is presented in terms of the hydraulic head in Figure 5 (second row). The results of the plume snapshots are presented in Figure 5 at 62, 620 and 3721 days since rclease. It is obvious that the plume at 62 is eloser to the left boundary in case of linear gradient while it left the domain completely after 3721 days in comparison with the radial flow case. This behaviour is due to the well effect as explained in the previous simulations.

C. 24



Figure 5. Simulation results in terms of piezometric head distribution and plume snapshots at three different times 62, 620 and 3721 days since release, top image is the heterogeneous aquifer (white is high permeable and black is low permeable). Left column is simulation under radial flow field and right column is simulation under linear gradient field.

The plume seennd moments are presented in Figure 6. In case of linear gradient flow tield the superdiffusive regime is observed as the case of perfectly layered formations. However in ease of radial flow, one can observe different regimes. In the first 500 days a subdiffusive regime is displayed. After the 500 days a superdiffusive regime is observed. The change of the regimes depends on the interaction between the alignment of the heterogeneity and the particle paths. In some places the particles accumulate causing subdiffusive regimes and in other cases particles move at high differential velocities between layers causing superdiffusive regimes. Modelling the behaviour of ehange from one regime to another is still a point of future research by the author.



Figure 6, Plume variance in case of slightly tilted formation under pure adavection.

6. CONCLUSIONS

In this paper, numerical simulations of a single-well tracer test in homogeneous, layered and slightly tilted aquifers under steady and axially symmetrical flow field from a fully penetrating injection well in a confined aquifer are developed. The simulations have been supplemented with analytical solutions for the evolution of the mean radial displacement of the tracer front and its variance due to pure advection in case of layered formations. A comparison with the case of linear gradient flow field is also considered.

The following conclusions can be drawn from this study:

- 1. If a tracer is injected into an axially symmetrical flow field in a layered system under advective transport the evolution of the mean of the tracer front is proportion to the square root of the travel time (Eq.10). While the variance of the front of the displacements is linearly proportion with travel time (Eq.11). This leads to a Fickian (diffusive) regime. The results show the discrepancies in the behaviour obtained from the case of uniform flow under linear hydraulic gradient, where non-Fickian (superdiffusive) regime is known [Mercado, 1967].
- 2. Excellent agreement exists between analytical solution and the numerical simulation for the case of pure advection in both first and second moments supporting the validity of the simulation.
- 3. In case of radial flow field, the arithmetic average conductivity is not a good representation of the layered medium as in the case of uniform flow under pure advection. However, the average of the square root of the hydraulic conductivity over the *n* layers, $\langle \sqrt{K_i} \rangle$ is the representative effective medium of the layered aquifer under axially symmetrical radial flow field.
- 4. The numerical experiment with particle model shows a subdiffusive dispersion regime in case of performing advection and dispersion in homogeneous aquifer under radial flow field condition due to the decline of the velocity from the well to the outer edge of the aquifer.
- 5. In case of slightly tilted formations, the change of the transport regimes depends on the interaction between the alignment of the heterogeneity and the particle paths. This behaviour needs further research developments.

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