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A SIMPLIFIED MODEL FOR TRANSPORT IN AQUIFERS

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ABSTRACT

Chemicals that are dissolved in groundwater flow along with the slow-moving water as it makes its way through the complex pores of the aquifer; during this process they are dispersed in different directions. The rate of dispersion depends on the porous structure and the fluid speed. Many groundwater aquifers have a natural layered structure; here this is used to advantage by discretizing them into "almost horizontal" layers, where each may have different matrix properties such as thickness, permeability, dispersivity, porosity, etc. The mean dynamic pressure (or mean hydraulic head) may be assumed constant vertically at each horizontal point if it is not in the vicinity of a well or where there is very small vertical flow. In the vicinity of recharge or pumping wells, the mean dynamic pressures or hydraulic heads for each sub-layer of the aquifer may be allowed to have different values for each different sub-layer. Steady-state fluid flow is considered here, in both confined and phreatic (unconfined) aquifers for illustration.

INTRODUCTION

Geological structures are generally composed of layered structures. The thickness of such sedimentary layers is very small compared to their lateral extent. Within each sub-layer the physical properties such as permeability, porosity and dispersivity can be assumed constant at each horizontal point. Then, partial differential equations (PDE's) for vertically-averaged fluid flow and contaminant transport may be written for each sub-layer of the aquifer. Thus, a full 3-dimensional simulation is reduced to its 2-dimensional analogue and these PDE's are for values at the vertical mid-points of each sub-layer. These models are therefore simplified models of the aquifer where the aquifer is discretized vertically, based on the natural layering of the geological structure.

Aquifers can be divided into two main types for modelling purposes; confined and phreatic (unconfined) aquifers. Confined aquifers have impermeable boundaries at both the top and the bottom. Phreatic aquifers do not have an impermeable top boundary and

hence the water table is free to move up when the aquifer is recharged naturally from surface water or artificially from a recharge well, and down when water is pumped out of the aquifer. The flow of fluid and transport of contaminants in confined and rigid aquifers where the thicknesses of the sub-layers are uniformly constant have been explored in [1]; there, the vertical flow of the isothermal and incompressible fluid is assumed to be very small and there are no sources or sinks to cause significant interlayer vertical flow

In the more general case when the thicknesses of the sub-layers of the confined aquifers are varying, the fluid flow and the tracer or contaminant transport model has been formulated in [2]. Fluid flowing in a layer may enter into neighbouring layers at a rate that depends on the difference of permeabilities and thicknesses of the two layers; again, the vertical flow was assumed negligible.

The model was extended to include fluid flow and tracer transport in phreatic aquifers in [3] and [4] by maintaining the assumption of no significant vertical flow. The difficulty of implementing numerical procedures when a sub-layer of the aquifer appears or disappears laterally (e.g. a lens) has been explored in [5]. It was found that by allowing the sub-layer with partial appearance to continue across the lateral extent of the aquifer with a very small thickness does not affect the total results. The removal of hazardous contaminants in groundwater by introducing strong oxidizers into the aquifer was discussed in [6]; there, a simple model based on the natural layering of the aquifer was used to model the flow of the introduced remediation agent in the groundwater while the pollution degradation takes place.

In all these models, vertical flow was assumed to be very small. In cases where there are recharge wells or pumping wells, vertical or interlayer flow is not purely based on the difference in permeabilities and thicknesses of the sub-layers. The mean dynamic pressure may not then be assumed constant throughout the thickness of the aquifer. This paper includes illustrations from previous models and some illustrations from the newer work when

each sub-layer of the aquifer has a different mean dynamic pressure from those above and below.

NOMENCLATURE

F = fluid recharge rate or pumping rate
 \bar{H} = mean hydraulic head
 h = thickness
 K = permeability
 \bar{P} = mean dynamic pressure
 q = total volume flux
 u = x -component of fluid speed
 v = y -component of fluid speed

Greek Symbols

α = dispersivity
 δ = Dirac delta function
 μ = fluid dynamic viscosity
 ρ = fluid density
 φ = porosity
 ψ = stream function

Subscripts

L = longitudinal
 P = pollutant
 R = remediating agent
 T = transverse

1 Fluid Flow

Mean dynamic pressure can be assumed constant vertically at each horizontal point (x, y) of the multi-layered aquifer if there is no significant vertical flow, or modelling is being done for a zone that is far from any recharge wells, pumping wells, etc., that may cause vertical flows ([1], [2], [3], [4], [5] and [6]). Wells that have perforations through the thickness of the whole aquifer do not cause significant vertical flow; therefore, this model is still useful for those cases.

The governing PDE for the mean dynamic (gauge) pressure \bar{P} in a confined aquifer composed of N sedimentary sub-layers each with thickness $h_i(x, y)$ and permeability $K_i(x, y)$, in the presence of a pumping well at (x_0, y_0) with pumping rate \bar{F}_p [$\text{m}^3 \text{s}^{-1} \text{m}^{-1} = \text{m}^2 \text{s}^{-1}$] of fluid per unit thickness of the aquifer and a recharge well at (x_1, y_1) with recharge rate \bar{F}_R [$\text{m}^2 \text{s}^{-1}$] of fluid per unit thickness, both averaged over the thickness, is found to be

$$\begin{aligned} & \frac{\partial}{\partial x} \left(h \bar{K} \frac{\partial \bar{P}}{\partial x} \right) + \frac{\partial}{\partial y} \left(h \bar{K} \frac{\partial \bar{P}}{\partial y} \right) \\ & = \mu h \bar{F}_p \delta(x - x_0) \delta(y - y_0) \\ & - \mu h \bar{F}_R \delta(x - x_1) \delta(y - y_1), \end{aligned} \quad (1)$$

where $h(x, y)$ is the total thickness of the aquifer, i.e., $h = \sum_{i=1}^N h_i$ and $\bar{K}(x, y)$ is weighted average of the permeabilities of all sub-layers, $\bar{K} = (\sum_{i=1}^N h_i K_i) / h$. Once the pressure field is found from (1) by using

suitable boundary conditions, the velocity field can be computed readily by using Darcy's law:

$$(\bar{u}_i, \bar{v}_i) = -\frac{K_i}{\mu} \left(\frac{\partial \bar{P}}{\partial x}, \frac{\partial \bar{P}}{\partial y} \right), \quad (2)$$

where $\bar{u}_i(x, y)$ is the component of fluid velocity in the x -direction and $\bar{v}_i(x, y)$ in the y -direction.

As a simple illustration, consider an aquifer consisting of only one (homogeneous) layer, as shown in Figure 1. The thickness profile for the aquifer is $h(x, y) = 1 + 0.5 \cos(\pi x / 25) \cos(\pi y / 20)$. There is a background steady flow due to a pressure gradient in the x -direction. Suppose that the aquifer is being recharged with a recharge well at $(40, 50)$ and water is being removed at $(80, 30)$ by a pumping well. The PDE in (1) is solved numerically with zero flux boundary conditions at $(x, 0)$ and $(x, 80)$ and with $\bar{P}(0, y) = 20$ [Pa] and $\bar{P}(100, y) = 0$ [Pa]. All other parameters are listed in Table 1.

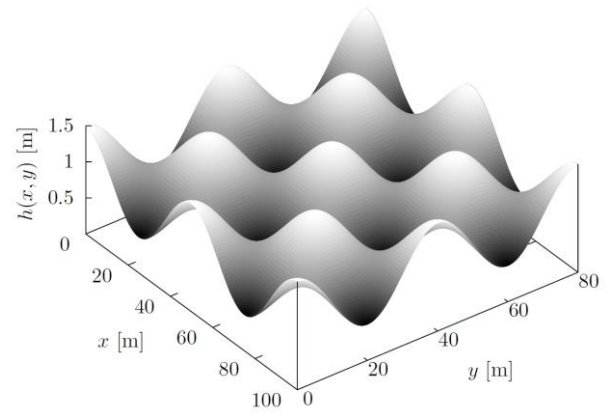


Figure 1: A rectangular homogeneous aquifer with a recharge well at $(40, 50)$ and a pumping well at $(80, 30)$. The thickness is shown; the base of the aquifer need not be planar. The slope in thickness is not as big as it looks here because of the exaggerated vertical scale.

The resultant isobars are plotted in Figure 2 in red. The isobars are contoured at an equal spacing between the highest and the lowest values of the mean dynamic pressure. For the values used for the boundary conditions and recharge and pumping rates, the highest value is at the recharge well and the lowest value at the pumping well.

Table 1: Parameters used to solve fluid flow in the aquifer shown in Figure 1.

parameter	value	unit
dynamic viscosity μ	0.001002	$\text{kg m}^{-1} \text{s}^{-1}$
permeability K	10^{-7}	m^2
recharge rate \bar{F}_R	86.4	$\text{m}^3 \text{day}^{-1} \text{m}^{-1}$
pumping rate \bar{F}_p	86.4	$\text{m}^3 \text{day}^{-1} \text{m}^{-1}$

The stream function $\psi(x, y)$ [$\text{m}^3 \text{s}^{-1}$] can be computed by integration in the y -direction of the x -component of the total volume flux, $q_x(x, y) = \bar{u}(x, y)h(x, y)$ [$\text{m}^2 \text{s}^{-1}$], as $\psi(x, y) = \int_0^y q_x dy$. The resultant stream function has discontinuities around the recharge and pumping wells on their downstream sides which are equal to the recharge and pumping rates, respectively.

The streamlines can be made to look continuous by joining streamlines with a difference equal to the recharge rate across the line of discontinuity caused by a recharge well, or equal to the pumping rate if the discontinuity is caused by a pumping well. The resultant continuous streamlines are also plotted in Figure 2 in blue. The amounts of fluid flowing between each pair of adjacent streamlines are equal and constant. The fluid that is being recharged at (40,50) pushes some of the background flowing fluid across to make its way. Some of the streamlines terminate at (80,30); this indicates that fluid is being pumped out of the aquifer from that point. Note that the stream function can also be computed by integrating the y -component of the total volume flux $q_y(x, y) = \bar{v}(x, y)h(x, y)$ in x -direction as $\psi(x, y) = \int_0^x q_y dx$. The stream function so computed will have discontinuities around recharge and pumping wells in the $+y$ -direction.

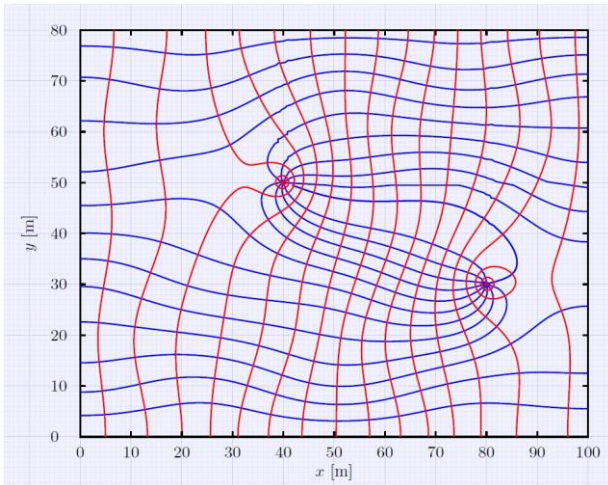


Figure 2: Isobars (red) and streamlines (blue) computed for the rectangular aquifer shown in Figure 1 with a recharge well at (40, 50) and a pumping well at (80, 30).

The fluid speed along the streamlines that originate from the recharge well and end at the pumping well is more than in the rest of the aquifer because of the steeper mean dynamic pressure gradient.

As another illustration, the next example is chosen for a layered phreatic aquifer consisting of four sedimentary sub-layers and an impermeable bottom, where fluid is being recharged (from a stream) in only one of the sub-

layers (the top layer) of the aquifer, as shown in Figure 3. It is convenient to model the mean hydraulic head instead of the mean dynamic pressure for fluid flow analysis in phreatic aquifers (e.g., [4]). It is clear that the hydraulic head cannot be assumed to be vertically constant at each horizontal point because interlayer vertical fluid flow occurs near the source because of the difference in pressures (or hydraulic heads).

The solution for the mean hydraulic heads in all the sub-layers is shown in red as a contour plot in the lower part of Figure 3. The computed head for each sub-layer is shown in the middle of that sub-layer. The fluid dynamic viscosity μ is the same as for the aquifer in Figure 1. The fluid density ρ is $1000 \text{ [kg m}^{-3}\text{]}$. The permeabilities in the sub-layers are $10^{-10} \times (0.7, 1.0, 0.5, 0.1) \text{ [m}^2\text{]}$ starting from the bottom. The boundary conditions for the mean hydraulic heads $\bar{H}_i(x)$ are $\bar{H}_1(0), \bar{H}_2(0), \bar{H}_3(0), \bar{H}_4(0) = 2.9 \text{ [m]}$ and $\bar{H}_1(10), \bar{H}_2(10), \bar{H}_3(10), \bar{H}_4(10) = 2.4 \text{ [m]}$, where the sub-layers are ordered from bottom to top. The water table in the stream is 2.7 as marked by a red solid line in Figure 3. The blue curve at the top is also the mean hydraulic head computed for the top sub-layer. This is the physical water table (also called the phreatic surface). The dotted blue line in the stream is the mean hydraulic head in the top sub-layer; it indicates that if a well was dug in the top sub-layer, water would achieve that level. The isobars are plotted at an equal spacing between the maximum mean hydraulic head (2.9 [m]) and the minimum mean hydraulic head (2.4 [m]).

The upper graph in Figure 3 is the total volume flux $q_x(x)$ [$\text{m}^3 \text{hr}^{-1} \text{m}^{-1}$] of fluid per unit width of the aquifer. Some water flow from the aquifer into the stream can be observed for some part of the stream as q_x drops for a while and then water enters into the aquifer where the mean hydraulic head of sub-layer 4 drops below the water table. The net overall increase in the value of q_x means more water enters the aquifer than leaves.

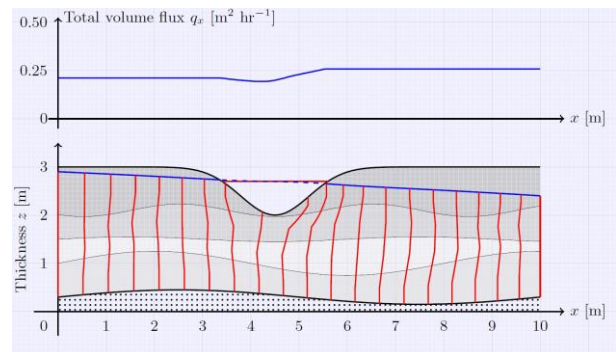


Figure 3: Isobars (lines of constant hydraulic head) computed in the layered phreatic aquifer with a transversely-running stream at the top. The water level in the stream is marked with a solid red horizontal line.

2 Pollutant Transport

Dissolved pollutants disperse in all directions when they move through the complex pores within the aquifer. The overall dispersion is the result of the two effects; molecular diffusion and mechanical dispersion. When polluted water makes its way through the heterogeneous pores, some of it shoots past the easy pathways but some of it finds it hard to pass through. Thus, the pollutant is dispersed mechanically on a longer distance along the direction of flow. In a direction transverse to the main flow direction, pollutant usually disperses on a smaller scale. The dispersion coefficient is suggested to be proportional to the fluid speed ([7]). If the x -axis of the Cartesian coordinate system is aligned with the main flow direction, the coefficient of dispersion along the main direction of flow is $D_x = \alpha_L |\mathbf{q}| / (\phi h)$ and the coefficient of dispersion along the transverse direction of flow is $D_y = \alpha_T |\mathbf{q}| / (\phi h)$, where α_L is usually larger than α_T . The constants α_L and α_T are called dispersion lengths or dispersivities. The pollutant also disperses in vertical directions from one sub-layer to the other. The model equations for multi-layered aquifers are shown by [2], [3], [4], [5] and [6].

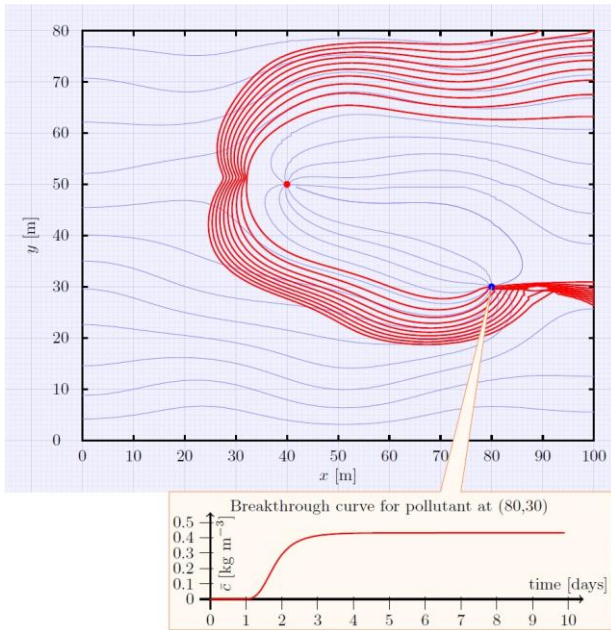


Figure 4: The computed pollutant concentration contours at steady state when water that is being injected through the well at (40,50) is polluted. The concentration of the pollutant at the pumping (monitoring) well becomes steady after a while as shown in the break-through curve (pop-out graph at the observation well).

As an illustration, consider that the fluid with which aquifer in Figure 1 is being recharged at (40,50) is contaminated with a concentration $c_R = 1$ [kg m⁻³]. The steady-state solution for the pollutant concentration in the aquifer is shown in Figure 4 as a contour plot. The contours are plotted at an equally spaced logarithmic scale $10^{-3}, -2.7, -2.4, \dots, 0$ from the outer contour to the inner one, respectively. The recharge well is marked with a

red circle and the pumping well is marked with a blue one. The longitudinal dispersivity α_L is taken as 1 [m] and the transverse dispersivity α_T is 0.1 [m] for this simulation. The porosity (the ratio of the void space in the porous medium to the total volume in a representative elementary volume) is 0.1 [-]. The breakthrough curve at the pumping well or monitoring well shows the concentration of the pollutant in the pumped-out water plotted against time. After almost 4 days, the concentration of the pollutant in pumped water reaches a steady level.

Some of clean water is also pumped out at the monitoring well; that is why the pollutant concentration of the pumped water is less than that of the middle of the concentration profile hump.

As an illustration for a layered phreatic aquifer, consider that the transverse running stream at the top of the aquifer shown in Figure 3 is polluted with concentration $c_R = 1$ [kg m⁻³]. It is assumed that the concentration of the pollutant in the stream water does not change significantly with the clean water that enters from the aquifer into the stream. The pollutant from the stream mixes with the slow-moving clean water of the aquifer. After a long time, the solution of the pollutant concentration reaches steady state, and this is shown in Figure 5 as a contour plot. The contours are plotted on an equally space logarithmic scale $10^{-2.5}, -2.3, -2.1, \dots, -0.1$ from the outer contour to the inner ones. The porosities of all the sub-layers are taken as 0.1 [-]. The longitudinal dispersivities used are (0.230, 0.250, 0.225, 0.200) [m] and the transverse (vertical) constant dispersion coefficients are (0.046, 0.050, 0.045, 0.040) [m² hr⁻¹] both in order from the bottom sub-layer to the top.

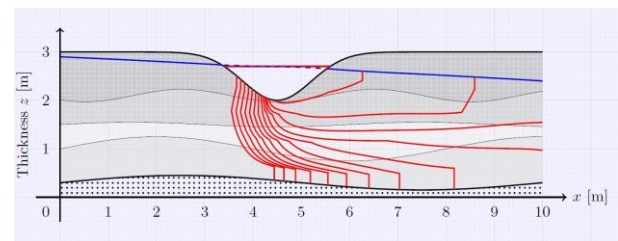


Figure 5: Contours of the steady-state pollutant concentration in the layered aquifer of Figure 3 when the stream water is uniformly contaminated.

3 Remediation

An illustration of the remediation model [6] is presented in this section. Consider again the aquifer shown in Figure 1 and assume a continuous injection of a strong oxidizer (a remediating agent) without significant fluid along with it at (50,50) just in front of the recharge well. The steady injection rate for the dry remediating agent is $q_R = 20$ [kg m⁻¹ day⁻¹]. The injected water at (40,50) is again contaminated with concentration $c_R = 1$ [kg m⁻³]. The steady-state solution for the pollutant concentration for this case is shown in Figure 6. The contours are

plotted on a logarithmic scale $10^{-3}, -2.7, -2.4, \dots, 0$ from the outer contour to the inner ones. The second-order decay rates for the pollutant and the remediating agents are $k_P = 5$ and $k_R = 1$ [$\text{kg m}^{-3} \text{day}^{-1}$], respectively. The longitudinal and transverse dispersivities for both the pollutant and the remediating agent are the same as for the simulation in Figure 4. The new breakthrough curve at the pumping well at (80,30) is plotted in solid red in the pop-out graph there. The dashed red curve is the breakthrough curve for a simulation without any added remediating agent. Another pop-out graph at (95,50) shows breakthrough curves for the pollutant at that point. The dashed red curve is the concentration of the pollutant at that point when there is no remediating agent being released, while the solid one is the breakthrough curve when the remediating agent is being released with rate q_R .

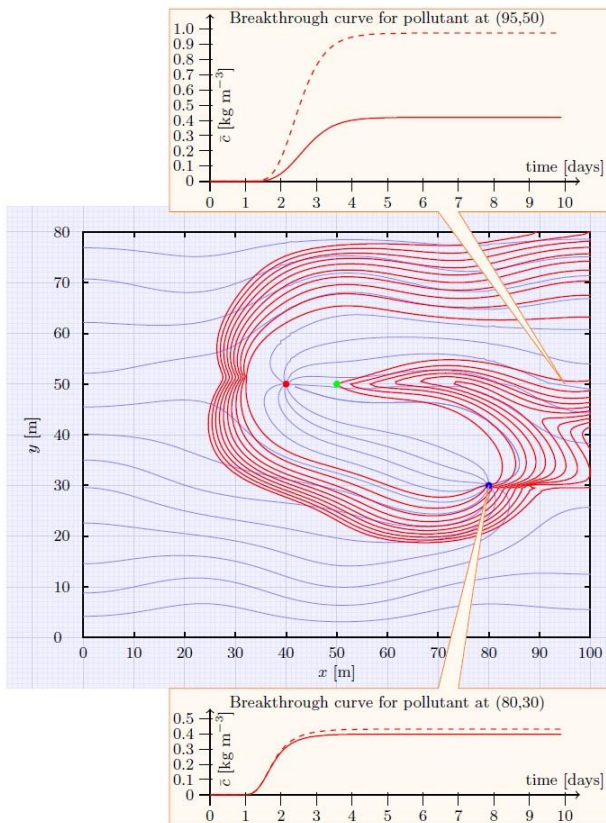


Figure 6: The concentration profile of the pollutant when the aquifer of Figure 1 is being recharged with contaminated water at (40,50) and a remediating agent is being released steadily at (50,50). Water is being through a pumping well located at (80,30). The fluid recharge rate, the fluid pumping rate and the remediating injection rates are given in the text.

It may be seen that there is a big difference between the removed steady concentration at (95,50) and that at the monitoring well at (80,30). As discussed above, the fluid speed between the recharge and the pumping well is much greater than that in rest of the aquifer. This does not allow the agent to co-exist with the pollutant for long

enough to make significant changes. However, the fluid carrying the remediating agent moves relatively slowly from the injection point of the remediating agent to (95,50) and hence there is more opportunity for the remediating agent to oxidize the pollutant.

Figure 7 shows the concentration profile of the remediating agent when it is being advected with the fluid, being dispersed in all directions and being used up to remove the pollutant. One can observe that the pollutant from the recharge well disperses more than the remediating agent from its injection point. This is because the fluid dispersing from the recharge well advects the pollutant along with it whereas the remediating agent does not have any fluid with it to alter the background fluid flow. Some of the remediating agent is also removed by the pumping well. So, in this case, the pumped out water contains concentrations of both the pollutant and the remediating agent.

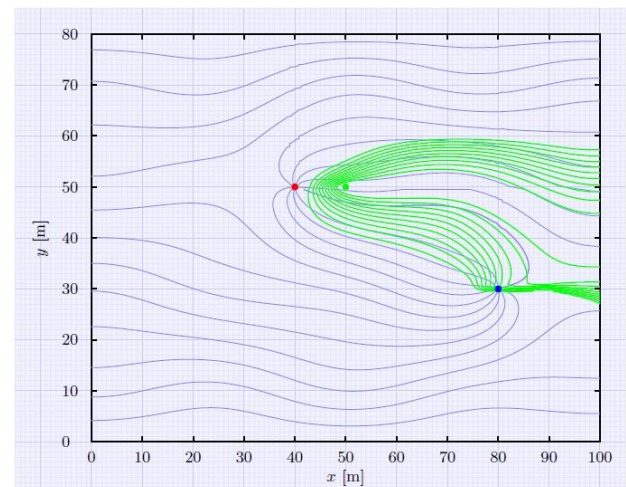


Figure 7: The concentration profile of the remediating agent.

CONCLUSIONS

In this paper, some simplified models have been presented for predicting pollutant concentration transported by groundwater flow within homogeneous or layered aquifers. The vertical discretization based on the natural layering of the geological structures simplifies the problem from a full-scale three-dimensional modelling of fluid flow and transport in each sub-layer to their two-dimensional averages. By solving fluid flow and transport models in each of the sub-layers and by matching the transfers at the sub-layer interfaces, the three-dimensional naturally-discretized (simplified) models have developed. The models can be used for any layered three-dimensional aquifer. The examples presented were chosen to be two-dimensional for better demonstration purposes.

Even if the sub-layers are not well-defined, the aquifer can still be discretized vertically and be treated in the same way as the geologically-stratified cases considered

above. The layering definition should be done in the best possible way so that the physical properties in each of the sub-layers do not vary much in the vertical direction at each horizontal point.

The presented remediation models [6] are for the remediation strategy called In Situ Chemical Oxidation (ISCO) and the reaction between the pollutant and the remediating agent has been taken as of second order. The exact order depends on the nature of the chemicals involved in the reaction. Similarly, the decay rates of the pollutant and the remediating agent used are only illustrative.

The governing equations for the mean hydraulic heads in a layered phreatic aquifer have not been presented because of space constraints. These equations and their background mathematics will be published at a later time.

REFERENCES

- [1] R. McKibbin, Groundwater pollutant transport: transforming layered models to dynamical systems, *An. St. Univ. Ovidius Constanta, Ser. Mat* **17**, pp 183-196 (2009).
- [2] R. McKibbin, Some aspects of modelling pollution transport in groundwater aquifers, in *Proceedings of CIAM 2010, Conference on Industrial and Applied Mathematics 6-8 July 2010, Institut Teknologi Bandung, Indonesia*, edited by L. H. Weiranto, and S. Pudjaprasetya, pp. 9-16, ISSN 977-208-70510-0-8 (CD) (2010).
- [3] A. Ali, R. McKibbin, and W.L. Sweatman, Simplified modelling of pollutant transport in stratified groundwater aquifers, in *Proceedings of International Congress on Environmental Modelling and Software Society (iEMSS) 2012, Managing Resources of a Limited Planet, Sixth Biennial Meeting, Leipzig, Germany*, edited by R. Seppelt, A. Voinov, S. Lange, and D. Bankamp, pp 2739-2746 (2012).
- [4] A. Ali, R. McKibbin, and W.L. Sweatman, Fluid flow and solute transport in unevenly-stratified groundwater aquifers, in *Proceedings of Porous Media and its Applications in Science, Engineering, and Industry, Fourth International Conference, Potsdam, Germany, June 17-22, 2012*, edited by K. Vafai, American Institute of Physics, 1453, pp 11-16, (2012).
- [5] A. Ali, R. McKibbin, and W.L. Sweatman, Tracer transport: appearing or disappearing sub-layers in a groundwater aquifer, in *Proceedings of 23rd International Symposium on Transport Phenomena, Auckland, New Zealand 19-22 November, 2012*, edited by Gordon Mallinson (2012).
- [6] A. Ali, W.L. Sweatman and R. McKibbin, Pollutant transport and its alleviation in groundwater aquifers, in M. Fontes, M. Günther, N. Marheineke (eds.), *Progress in Industrial Mathematics at ECMI 2012*, Mathematics in Industry 19, Springer Berlin Heidelberg, [ISBN 978-3-319-05365-3 (ebook), ISBN 978-3-319-05364-6 (hardcover)] (in press, 2014)
- [7] J. Bear, and A. Verruijt, *Modeling groundwater flow and pollution*, D. Reidel, Dordrecht, Holland, 1978.