

Simplified Modelling of Pollutant Transport in Stratified Groundwater Aquifers

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Abstract: Chemical species such as tracers or dissolved pollutants are dispersed by water flowing within a permeable matrix. The species move not only “down-stream”, but also spread in all directions. The rate of dispersion depends on the permeability structure and the fluid speed. Generally, groundwater systems have layered structures determined by different events in the geological processes that formed them. The layers in a system have different physical properties, and their thicknesses are not uniform. The system of advection-dispersion equations that model the fluid and species transport then have coefficients that depend mainly on depth, but with a layer composition that may change with horizontal distance. A single-layered homogeneous, confined aquifer is considered first, where the matrix and flow parameters are assumed constant. The aquifer thickness is assumed small compared to its lateral extent, and slopes of its boundaries are also small. The steady-state fluid flow and the associated pressure distribution may be readily computed. The vertically-averaged pollutant concentration within the single-layered aquifer varies in the plane of the flow; lateral changes in concentration within the aquifer may occur by advection and dispersion. The idea is extended to multi-layered non-homogeneous aquifers where each layer may have properties different from the others. In some cases, full or partial analytic solutions for the species concentration can be found, thereby saving computational effort.

Keywords: mathematical modelling; groundwater; aquifers; pollutant; dispersion; permeability

1 INTRODUCTION

The dispersion of dissolved contaminants when they are advected in stratified groundwater aquifers where the different sedimentary layers are parallel and horizontal, has been explored by McKibbin [2009]. In this work, thicknesses of different layers are no longer considered constant. In addition to the dispersive transfer of pollutant from one layer to its neighbour(s), fluid flux through the layer interfaces may also occur; this depends on the thicknesses and the permeabilities of the neighbouring layers and the slope of the interfaces. This fluid carries (advects) dissolved pollutant with it across the layer interface.

The fluid flow is assumed steady, while the contaminant is assumed to be soluble and non-reacting. The thickness profiles of the different sedimentary layers vary slowly spatially. Commonly, the thickness of an aquifer is very small compared to its lateral extent (Bear and Bachmat [1991]). The governing equations for the fluid flow are developed for a multi-layered aquifer with this assumption that the horizontal gradients of the layer interfaces are small.

The coupled mass-balance equations for multi-layered aquifer systems were formulated by McKibbin [2010]. Some illustrative examples are presented in this paper.

2 FLUID FLOW MODEL FOR A CONFINED AQUIFER

The Darcy velocity within an isotropic porous medium in a Cartesian coordinate system (x, y, z) , where z is vertical, is given by the famous Darcy's law:

$$\vec{u}(x, y, z) = \frac{K}{\mu} (-\nabla p + \rho \vec{g}) = \frac{K}{\mu} (-\nabla P), \quad (1)$$

where K [L^2] is the permeability of the porous structure, μ [$M L^{-1} T^{-1}$] is the dynamic viscosity of the fluid, p [$M L^{-1} T^{-2}$] is the absolute pressure in the fluid, ρ [$M L^{-3}$] is the fluid density, $\vec{g} = (0, 0, -g)$ [$L T^{-2}$] is the gravitational acceleration, and P is the fluid dynamic pressure given by $P(x, y, z) = p(x, y, z) - p_0 + \rho g z$, where p_0 is a datum pressure. From mass conservation, the Darcy velocity \vec{u} of an incompressible and isothermal fluid in a rigid porous media is a solenoidal vector, i.e., $\nabla \cdot \vec{u} = 0$.

Suppose that the fluid is flowing in a confined aquifer composed of N sedimentary layers, which may have matrix properties that are different from each other. Within a layer the matrix properties are assumed to be similar at different heights although they may vary slowly in the horizontal directions. The thicknesses of the layers may also vary with horizontal position (x, y) . The layer interface levels at horizontal position (x, y) are denoted by $z_0(x, y), z_1(x, y), z_2(x, y), \dots, z_N(x, y)$, with $z_0(x, y)$ and $z_N(x, y)$ being the impervious bottom and top boundaries of the aquifer, respectively. Then the thickness of the i th layer is $h_i(x, y) = z_i(x, y) - z_{i-1}(x, y)$, $1 \leq i \leq N$.

If the component of the Darcy velocity in the x -direction at point (x, y, z) of the i th layer of the aquifer is denoted $u(x, y, z)$, then the averaged horizontal speed of the fluid in the x -direction in the i th layer is

$$\bar{u}_i(x, y) = \frac{1}{h_i(x, y)} \int_{z_{i-1}(x, y)}^{z_i(x, y)} u(x, y, z) dz$$

at point (x, y) on the XY -plane. The total volume flux q_{x_i} per unit width of the i th layer in the x -direction is

$$q_{x_i} = h_i(x, y) \bar{u}_i(x, y) = \int_{z_{i-1}(x, y)}^{z_i(x, y)} u(x, y, z) dz. \quad (2)$$

Similarly, the total volume flux q_{y_i} in the y -direction through the i th layer can be written in terms of y -component v of the Darcy velocity. The horizontal (two-dimensional) total volume flux vector through the i th layer is then $\vec{q}_i(x, y) = (q_{x_i}(x, y), q_{y_i}(x, y))$, and the total horizontal volume flux vector through the whole aquifer is

$$\vec{q}(x, y) = (q_x(x, y), q_y(x, y)) = \sum_{i=1}^N (q_{x_i}(x, y), q_{y_i}(x, y)). \quad (3)$$

By applying the general form of the Leibniz integral rule and also continuity requirements of the fluid flux across the layer interfaces, it can be shown that

$$\nabla \cdot \vec{q} = \vec{u}_0 \cdot \nabla \phi_0 - \vec{u}_N \cdot \nabla \phi_N = 0. \quad (4)$$

Here, \vec{u}_0 and \vec{u}_N are the fluid specific discharges at z_0 and z_N , respectively. The functions ϕ_0 and ϕ_N are defined by $\phi_0(x, y, z) = z - z_0(x, y)$ and $\phi_N(x, y, z) = z - z_N(x, y)$, respectively. (Note that the bottom and top boundaries of the confined aquifer system at

z_0 and z_N are assumed to be impervious; therefore the fluid velocity \vec{u} is parallel to these boundaries.)

The (two-dimensional) divergence of the horizontal volume flux through the i th layer is

$$\nabla \cdot (q_{x_i}, q_{y_i}) = \vec{u}_{i-1} \cdot \nabla \phi_{i-1} - \vec{u}_i \cdot \nabla \phi_i = r_{i-1}(x, y) - r_i(x, y); \quad 1 \leq i \leq N \quad (5)$$

Here, $r_i = \vec{u}_i \cdot \nabla \phi_i$ is the component of the fluid flux normal to the layer interface from the i th layer to the $i + 1$ th layer. The normal interface fluxes $r_0(x, y)$ and $r_N(x, y)$ are zero, because the bottom and the top boundaries of the aquifer are impervious. The averaged dynamic pressure in the i th layer over the layer thickness \bar{P}_i is defined by

$$h_i(x, y) \bar{P}_i(x, y) = \int_{z_{i-1}(x, y)}^{z_i(x, y)} P(x, y, z) dz.$$

Taking the partial derivative with respect to x and using Darcy's law for the x -component of the fluid specific discharge, it can be shown that

$$h_i \frac{\partial \bar{P}_i}{\partial x} = -\frac{\mu}{K_i} h_i \bar{u}_i + (P_i - \bar{P}_i) \frac{\partial z_i}{\partial x} - (P_{i-1} - \bar{P}_i) \frac{\partial z_{i-1}}{\partial x}, \quad (6)$$

where $P_i = P(x, y, z_i(x, y))$ is the dynamic pressure at the layer interface. Similarly, in the y -direction

$$h_i \frac{\partial \bar{P}_i}{\partial y} = -\frac{\mu}{K_i} h_i \bar{v}_i + (P_i - \bar{P}_i) \frac{\partial z_i}{\partial y} - (P_{i-1} - \bar{P}_i) \frac{\partial z_{i-1}}{\partial y}. \quad (7)$$

The vertical component of the Darcy velocity in layer i averaged over the layer thickness is

$$\bar{w}_i = \frac{1}{h_i} \int_{z_{i-1}}^{z_i} w(x, y, z) dz,$$

Then the vertical volume flux through the i th layer of the aquifer is

$$q_{z_i} = h_i \bar{w}_i = \int_{z_{i-1}}^{z_i} w(x, y, z) dz = \int_{z_{i-1}}^{z_i} \frac{K_i}{\mu} \left(-\frac{\partial P}{\partial z} \right) dz = \frac{K_i}{\mu} (P_{i-1} - P_i). \quad (8)$$

Rearranging the mass conservation equation $\nabla \cdot \vec{u} = 0$, we have

$$\frac{\partial w}{\partial z} = -\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right). \quad (9)$$

If horizontal variations in pressure in the i th layer are $O(\Delta P_i)$, then the horizontal components of fluid velocity in the i th layer (and mean horizontal fluid velocities \bar{u}_i, \bar{v}_i in each layer) are of order $(K_i \Delta P_i) / (\mu L)$, where L is the order of the lateral extent of the aquifer. If the thickness of the i th layer of the aquifer is $O(H_i)$, then horizontal gradients of the i th layer interfaces are $O(\epsilon_i)$, where $\epsilon_i = H_i / L \ll 1$ and (9) shows that w_i (and \bar{w}_i) is $O((\epsilon_i K_i \Delta P_i) / (\mu L))$. Also, (8) shows that vertical variations in P in the i th layer are $O((\mu H_i \epsilon_i K_i \Delta P_i) / (K_i \mu L)) = O(\epsilon_i^2 \Delta P_i)$. Thus, the latter two terms of both (6) and (7) are a factor $O(\epsilon_i^2)$ smaller than the corresponding first right-hand terms, and they may be neglected for small ϵ_i . The mean dynamic pressure over whole aquifer thickness is then $\bar{P} = \left(\sum_{i=1}^N h_i \bar{P}_i \right) / h$, where $h(x, y) = \sum_{i=1}^N h_i(x, y)$.

The continuity requirement for P at the layer interfaces implies that vertical variations in \bar{P}_i are $O\left(\sum_{i=1}^N \epsilon_i^2 \Delta P_i\right)$. So, to a good approximation, \bar{P}_i in (6) and (7) may be replaced with \bar{P} , and therefore

$$\frac{\partial \bar{P}}{\partial x} = -\frac{\mu}{K_i} \bar{u}_i, \quad \frac{\partial \bar{P}}{\partial y} = -\frac{\mu}{K_i} \bar{v}_i. \quad (10)$$

The mean horizontal velocity components in each layer may then be written as

$$(\bar{u}_i, \bar{v}_i) = -\frac{K_i(x, y)}{\mu} \left(\frac{\partial \bar{P}}{\partial x}, \frac{\partial \bar{P}}{\partial y} \right). \quad (11)$$

Using (2) and (11) in (3), it is found that

$$(q_x(x, y), q_y(x, y)) = -\left(\sum_{i=1}^N h_i(x, y) K_i(x, y) \right) \frac{1}{\mu} \left(\frac{\partial \bar{P}}{\partial x}, \frac{\partial \bar{P}}{\partial y} \right). \quad (12)$$

Now, using (12) in (11) and the result in (2), the layer total volume fluxes can be written as

$$(q_{x_i}, q_{y_i}) = \frac{h_i(x, y) K_i(x, y)}{\sum_{j=1}^N h_j(x, y) K_j(x, y)} (q_x, q_y). \quad (13)$$

If the horizontal components of the fluid velocity averaged over the whole aquifer system thickness in the x and y -directions are denoted by $\bar{u}(x, y)$ and $\bar{v}(x, y)$ respectively, then (4) gives

$$\frac{\partial}{\partial x} (h(x, y) \bar{u}(x, y)) + \frac{\partial}{\partial y} (h(x, y) \bar{v}(x, y)) = 0, \quad (14)$$

Equation (14) suggests defining a stream function $\psi(x, y)$ [$L^3 T^{-1}$] through the whole aquifer by

$$h(x, y) \bar{u}(x, y) = \frac{\partial \psi}{\partial y}, \quad h(x, y) \bar{v}(x, y) = -\frac{\partial \psi}{\partial x}. \quad (15)$$

Using the condition of irrotationality of the fluid, $\partial \bar{u} / \partial y - \partial \bar{v} / \partial x = 0$, it can be shown that

$$\frac{\partial}{\partial x} \left(\frac{1}{h} \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{1}{h} \frac{\partial \psi}{\partial y} \right) = 0. \quad (16)$$

Also, using (12), (4) can be re-written as

$$\frac{\partial}{\partial x} \left(\sum_{i=1}^N (h_i K_i) \frac{\partial \bar{P}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\sum_{i=1}^N (h_i K_i) \frac{\partial \bar{P}}{\partial y} \right) = 0. \quad (17)$$

Defining vertically averaged permeability \bar{K} throughout the aquifer at each planar point (x, y) as $\bar{K}(x, y) = \left(\sum_{i=1}^N h_i K_i \right) / h$, equation (17) becomes

$$\frac{\partial}{\partial x} \left(h \bar{K} \frac{\partial \bar{P}}{\partial x} \right) + \frac{\partial}{\partial y} \left(h \bar{K} \frac{\partial \bar{P}}{\partial y} \right) = 0. \quad (18)$$

2.1 Example

For suitable boundary conditions, the mean dynamic pressure and the stream function can be found for an aquifer by solving (16) and (18) numerically (here, a finite-difference scheme is used). A simple example is used for illustration. A homogeneous aquifer lies in the rectangular region $0 \leq x \leq 100$, $0 \leq y \leq 80$, with the thickness profile $h(x, y) = 1 + 0.5 \cos(\pi x/25) \cos(\pi y/20)$. The boundary conditions are taken to be

$$\begin{aligned} \psi(x, 0) = 0, \quad \psi(x, 80) = 1, \quad \frac{\partial \psi(0, y)}{\partial x} = \frac{\partial \psi(100, y)}{\partial x} = 0, \quad \text{and} \\ \bar{P}(0, y) = 1, \quad \bar{P}(100, y) = 0, \quad \frac{\partial \bar{P}(x, 0)}{\partial y} = \frac{\partial \bar{P}(x, 80)}{\partial y} = 0. \end{aligned}$$

The thickness profile is shown in Figure 1(a) and the isobars and streamlines are plotted in Figure 1(b). Note that SI units are used in all the illustrative examples shown here.

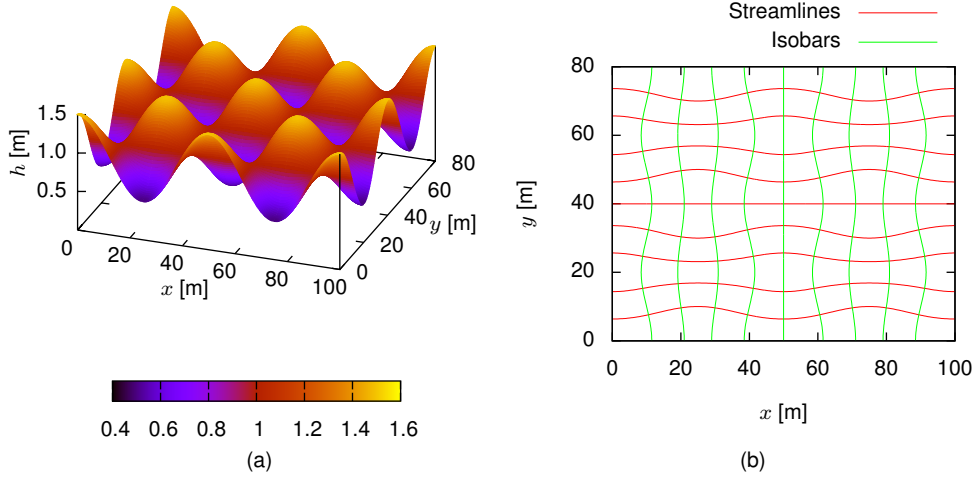


Figure 1: (a) Note that the bottom surface of the aquifer, here shown parallel to the XY -plane, need not be planar; this is just a special case of the thickness profile. (b) Streamlines and isobars. Note that streamlines and isobars are orthogonal wherever they intersect.

3 POLLUTION TRANSPORT MODEL FOR A CONFINED AQUIFER

In general, the model can be used to estimate pollutant concentrations in an aquifer consisting of N layers. If $\bar{f}_i(x, y, t)$ [$M L^{-3} T^{-1}$] is a distributed or a point source averaged over the layer thickness in the i th layer, then the layer-averaged pollutant concentration $\bar{c}_i(x, y, t)$ [$M L^{-3}$] in i th layer, which has porosity ϕ_i [-], thickness $h_i(x, y)$, and horizontal dispersion coefficient D_{H_i} [$L^2 T^{-1}$], satisfies (McKibbin [2010])

$$\begin{aligned} \phi_i h_i \frac{\partial \bar{c}_i}{\partial t} &= \frac{\partial}{\partial x} \left[-q_{x_i} \bar{c}_i + \phi_i D_{H_i} \frac{\partial \bar{c}_i}{\partial x} \right] + \frac{\partial}{\partial y} \left[-q_{y_i} \bar{c}_i + \phi_i D_{H_i} \frac{\partial \bar{c}_i}{\partial y} \right] \\ &+ \left[\tau_{i-1} + \frac{1 + \text{sgn}(r_{i-1})}{2} r_{i-1} \right] \bar{c}_{i-1} + \left[-\tau_{i-1} + \frac{1 - \text{sgn}(r_{i-1})}{2} r_{i-1} \right] \bar{c}_i \\ &+ \left[-\tau_i - \frac{1 + \text{sgn}(r_i)}{2} r_i \right] \bar{c}_i + \left[\tau_i - \frac{1 - \text{sgn}(r_i)}{2} r_i \right] \bar{c}_{i+1} \\ &+ \phi_i h_i \bar{f}_i(x, y, t), \end{aligned} \quad (19)$$

where $\tau_i(x, y)$ is the interlayer transfer coefficient between layer i and $i + 1$, given by

$$\frac{1}{\tau_i} = \frac{h_i/2}{\phi_i D_{V_i}} + \frac{h_{i+1}/2}{\phi_{i+1} D_{V_{i+1}}}, \quad (20)$$

and D_{V_i} is the coefficient of vertical dispersion in the i th layer. As discussed above, the interlayer flux $r_i(x, y)$ normal to the layer interface from the i th layer to the $i + 1$ th layer is given by (5). Equations (19) (with (20)) are N coupled partial differential equations and can generally be solved numerically with suitable boundary conditions.

3.1 Illustrations

Consider Q_m [$kg m^{-1}$] pollutant injected at $(x_0, y_0) = (10, 40)$ as a vertical line source at time $t = 0$ in a rectangular homogeneous aquifer with thickness profile $h(x, y) = 1 + 0.5 \cos(\pi x/25) \cos(\pi y/20)$; $0 \leq x \leq 100, 0 \leq y \leq 80$. The dispersion coefficient $D(x, y)$ is taken to be proportional to the mean interstitial fluid speed $|\bar{U}| = |\bar{u}/\phi|$, and is

assumed isotropic, with the same dispersion length α in both the lateral and transverse directions of the flow (van Herwaarden [1994]). Then

$$D(x, y) = \frac{\alpha}{\phi} \sqrt{\bar{u}^2 + \bar{v}^2}.$$

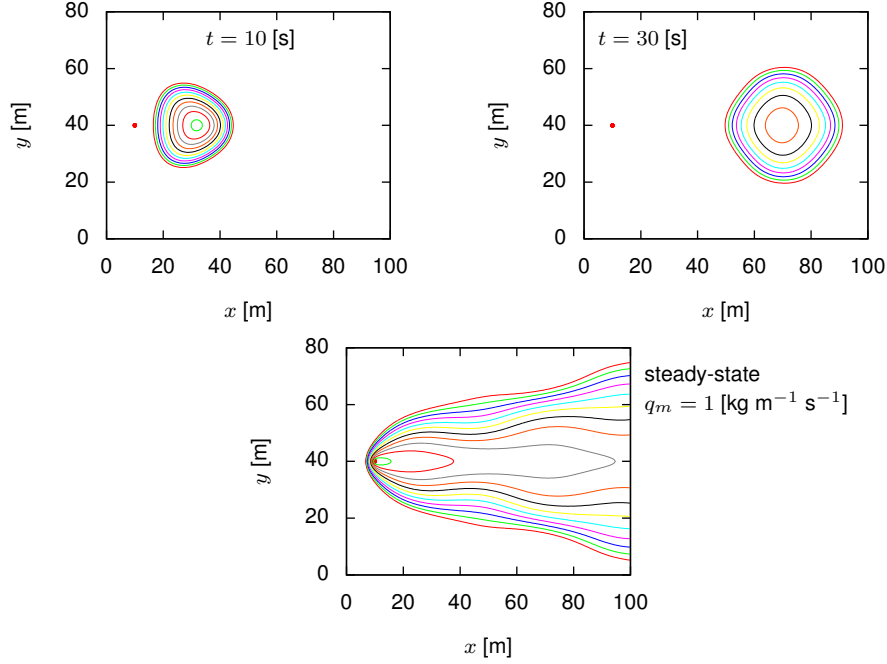


Figure 2: Snapshot of pollutant concentration at times t_1 and $t_2 = 3t_1$ after release $Q_m = 1$ as a vertical line source (marked as \bullet) in top left and right plots, respectively. The contours are plotted at the same levels from the outer contour to the inner ones on an equally-spaced logarithmic scale. The bottom plot is the steady-state pollutant concentration when it is released continuously at a constant rate q_m . The contours are again plotted on an equally-spaced logarithmic scale. The parameter values used are: $\alpha = 0.5$, $\phi = 0.1$, $P(0, y) = 10$, $P(L, y) = 0$, $K/\mu = 2$ (all units are given in the text).

The vertically-averaged pollutant concentration contours at times $t_1 = 10$ [s] and $t_2 = 30$ [s] after release are plotted in the top left and top right of Figure 2, respectively. For the case where the injection is continuous at a rate $q_m = 1$ [$\text{kg m}^{-1} \text{s}^{-1}$], the steady-state concentration contours are plotted in the bottom plot in Figure 2.

The next example compares pollutant flow in a confined homogeneous aquifer of varying thickness to that in a nonhomogeneous confined aquifer consisting of three layers with the middle layer more permeable than other two. Except for the permeability value of the middle layer of the nonhomogeneous aquifer, the total thickness of the two aquifers and all other parameters are the same. The total volume flux per unit aquifer width through each of the two systems has the same value ($1 \text{ m}^2 \text{ s}^{-1}$). Equal masses of pollutant are released as instantaneous sources at the same point in both cases. Both aquifers are discretized further into sub-layers (20 layers for both aquifers) and model (19) is used to predict pollutant concentration at times $t_1 = 0.5$ [s] and $t_2 = 1$ [s]. The “point source” is equivalent to a planar strip source for the model here. The resultant pollutant concentration contours are shown in Figure 3. In the middle higher-permeability layer the pollutant moves faster than in the neighbouring layers.

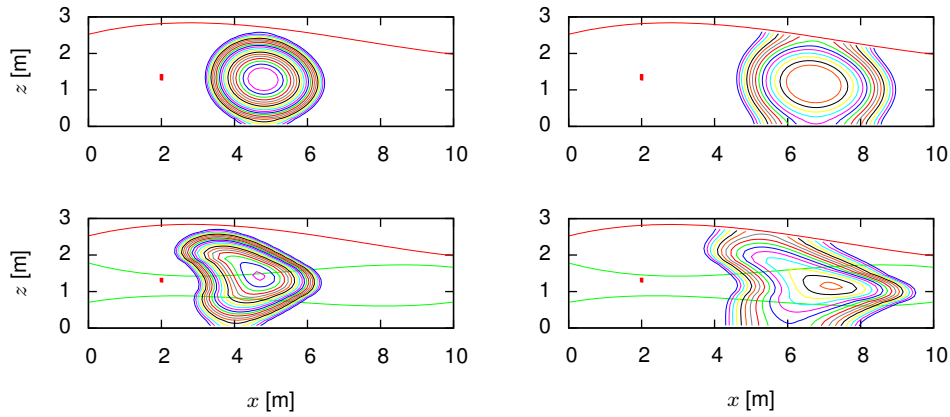


Figure 3: Pollutant concentration at times t_1 and $t_2 (=2t_1)$ after release as a planar strip source (indicated by a red rectangle) in two different aquifers. The parameter values for the homogeneous aquifer (upper plots) are: $\phi = 0.1$, $K = 1$, $D_H = 0.4$, $D_V = 0.25$, $q_x = 1$. The parameter values for the lower aquifer are the same except for the middle layer which is more permeable with $K = 2$ (all units are given in the text). The contours are plotted at the same levels from outer contours to the inner ones on an equally-spaced logarithmic scale.

The case where a uniformly-distributed source is released over a finite period of time into the top of a homogeneous confined aquifer is shown in Figure 4.

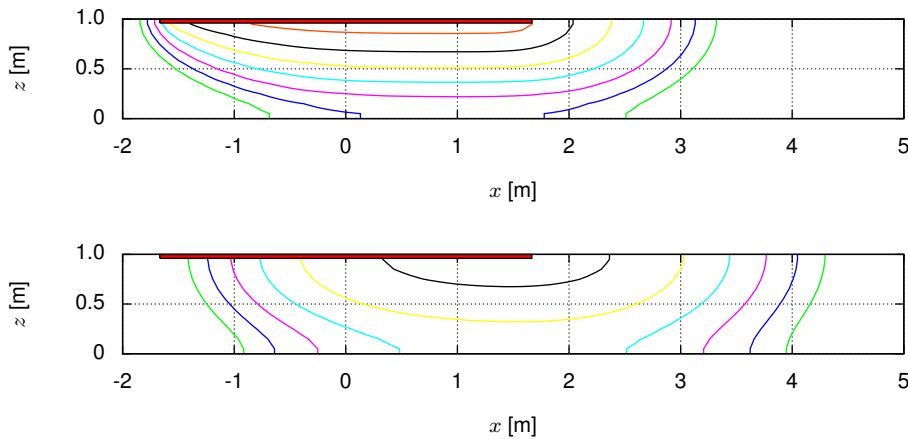


Figure 4: Confined aquifer. The region of pollutant release is marked as a horizontal thick bar at the top; the release has a duration of 1[s]. Concentration contours as predicted by the model are shown for the times $t = 1.2$ and $t = 2.0$ [s]. The parameter values are: $q_x = 0.1$, $q_m = 1$, $D_H = 0.15$, $D_V = 0.05$, $\phi = 0.1$ (all units are given in the text). The contours are plotted from the outer contour to the inner ones on an equally-spaced logarithmic scale.

4 PHREATIC AQUIFERS

Most fluid flow concepts are similar in phreatic (unconfined) aquifers to those for confined aquifers. They differ in that the shape of the phreatic surface must be determined. The Dupuit assumption is used for this and to find the points where the phreatic surface passes through layer interfaces. Due to space constraints, the calculation is omitted, however, an illustration is shown in Figure 5.

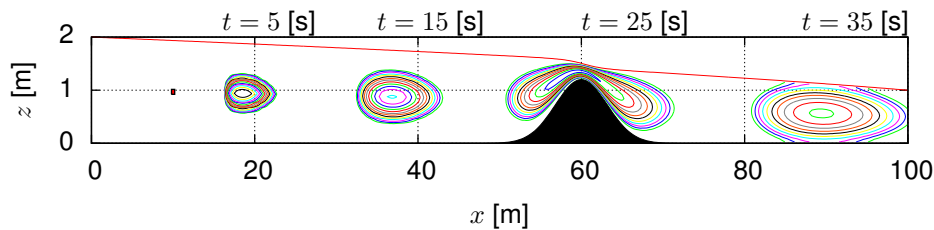


Figure 5: Unconfined (phreatic) aquifer. Pollutant transport as a result of an instantaneous release $Q_m = 1$ [kg m⁻²] as a planar strip source (indicated as a red rectangle). Concentration contours are plotted at times $t = 5, 15, 25, 35$ [s] after release. The parameters values are: $\phi = 0.3$, $D_H = 0.1$, $D_V = 0.001$, $q_x = 1$. The contours are plotted from the outer contour to the inner ones on an equally-spaced logarithmic scale. The phreatic surface is shown as a red curve.

5 SUMMARY

This paper describes fluid flow and pollutant transport models for confined and phreatic aquifers composed of layers that are of non-uniform thickness. The permeable matrix parameters are assumed constant within each layer vertically, but they are allowed to vary laterally. The model equation (19) can be used for vertical discretization of both homogeneous aquifers and nonhomogeneous aquifers. More generally, for nonhomogeneous aquifers where sub-layer thicknesses also vary, the layered model (19) can be used effectively.

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