



GROUNDWATER POLLUTANT TRANSPORT: TRANSFORMING LAYERED MODELS TO DYNAMICAL SYSTEMS

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Abstract

Chemical species such as tracers or dissolved pollutants disperse as they are advected by a fluid flowing within a permeable matrix. In many groundwater systems, the porous media have (near-horizontal) layered structures that have been determined by the geological processes which formed them. The advection-dispersion equations that model the transport then have coefficients that depend mainly on depth.

In this study, the parameters that contribute to the coefficients in the partial differential equations are assumed constant within each layer, but can be different in each of the various layers. This allows aquifer systems with parallel-bedded structures to be modelled without having to resort to full numerical simulations. Anisotropy in permeability and in the dispersive length scales, as well as removal of the chemical by adsorption onto the matrix surface and movement into and/or out of dead-end pores, may all be incorporated. The resulting linear constant-coefficient pde's are coupled by mass flux continuity requirements at the layer interfaces.

In many cases, full or partial analytic solutions for the species concentration can be found, thereby saving computational effort. The use of integral transforms, Green's functions and other techniques are used to solve the system of differential equations.

First, the equations that describe the movement of the fluid and pollutant species are summarized. The modelling device of images is

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then used to provide an analytical solution for species released into a homogeneous layer. This is followed by a derivation of the model equations for a multi-layered system; Fourier transforms allow conversion to a dynamical system that is partly solved analytically using standard techniques. The layered system may also be used as an approximate realization of an aquifer with properties that vary smoothly with depth. Some examples are given.

1 Introduction

The aim of this study is to mathematically model the transport of a pollutant injected into a groundwater aquifer that is composed of several different parallel sedimentary layers, where the layer thicknesses are assumed small compared to the lateral extent of the aquifer. The groundwater flow throughout is assumed to be under the influence of a uniform pressure gradient parallel to the layers. Within each layer, the pollutant concentration varies in the plane of the flow, but at each point is assumed to be nearly uniform through the layer perpendicular to the flow. Transfer of the pollutant across the layer interfaces may occur when the concentrations within adjoining layers are not equal.

The resulting mathematical model is a set of coupled linear time-dependent advection-dispersion equations. Fourier transforms (FT's) are applied with respect to the spatial variables; the resulting set of coupled linear first-order ordinary differential equations for the (complex-valued) pollutant concentration transforms (in time, and carrying the FT parameters) may then be solved using standard linear dynamical system techniques. The predicted pollutant concentrations are efficiently retrieved by numerically evaluating the inverse transforms.

The technique of using a layered model, either in its own right or as an approximate analogue of a continuous system, has been explored in other contexts. For example, [McKibbin & O'Sullivan(1981)] and [McKibbin(1992)] investigated thermally-driven convection in layered porous media.

[Lim *et al.*(2008)] and [McKibbin(2008)], using Green's functions, found analytic expressions for the airborne concentration and ground deposits of volcanic ash that falls through a stratified atmosphere. The application, as described below, of transforms to a system of coupled advection-dispersion equations is, to the author's knowledge, innovative and not used in the current context before.

2 The equations

A general derivation of the equations and discussion of the parameters is given, for example, in [Bear(1972)]. For isothermal, single-phase flow in a stationary porous medium, the momentum conservation equation (Darcy's law) is of the form:

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu}\nabla(p + \rho gz) \quad (1)$$

where, in the Cartesian coordinate system (x, y, z) [dimension: m] with the z -axis vertical upwards, $\mathbf{q} = (u, v, w)$ is the specific volume flux of the fluid $[(\text{m}^3 \text{ s}^{-1})/\text{m}^2 = \text{m s}^{-1}]$ (the so-called Darcy velocity), \mathbf{k} is the permeability tensor $[\text{m}^2]$, μ is the dynamic viscosity of the fluid $[\text{kg m}^{-1} \text{ s}^{-1}]$, p is the absolute pressure $[\text{Pa} = \text{kg m}^{-1} \text{ s}^{-2}]$, ρ is the uniform and constant fluid density $[\text{kg m}^{-3}]$ and g is gravitational acceleration $[\text{m s}^{-2}]$. The (second-order) permeability tensor is symmetric. If the permeability is assumed to be horizontally isotropic, the principal directions are aligned with the Cartesian coordinate axes, and the horizontal and vertical permeability components vary only with depth, then the tensor takes the form:

$$\mathbf{k} = \begin{bmatrix} k_H(z) & 0 & 0 \\ 0 & k_H(z) & 0 \\ 0 & 0 & k_V(z) \end{bmatrix} \quad (2)$$

If the pressure is hydrostatic and the horizontal component of the pressure gradient is constant and aligned with the x -axis, then $p = p_a - G(x - x_a) - g(z - z_a)$ [where subscript "a" refers to some datum, with $p(x_a, y, z_a) = p_a$], and $v = w = 0$. Equation (1) gives:

$$\frac{u}{k_H(z)} = \left(-\frac{1}{\mu} \frac{\partial p}{\partial x} \right) = \frac{G}{\mu} = \text{constant} \quad (3)$$

thereby determining the horizontal speed profile of the fluid. The conservation of mass of the fluid, which is assumed to contain only very small amounts (mass/mass) of the pollutant, is expressed by

$$\frac{\partial(\phi\rho)}{\partial t} + \nabla \cdot (\rho\mathbf{q}) = \phi \left(\frac{\partial\rho}{\partial t} + \frac{\mathbf{q}}{\phi} \cdot \nabla\rho \right) + \rho\nabla \cdot \mathbf{q} = \phi \frac{D\rho}{Dt} + \rho\nabla \cdot \mathbf{q} = 0 \quad (4)$$

where ϕ [-] is the porosity of the matrix. Here, $D\rho/Dt$ is the so-called material or Lagrangian derivative of the density. In the case where the fluid is liquid water, it may be assumed uniform and incompressible, in which case $D\rho/Dt = 0$, and then $\nabla \cdot \mathbf{q} = 0$.

The mass flux of a pollutant species per unit area of the fluid-saturated matrix has advective and dispersive components. The latter is modelled here as mechanical Fickian-type dispersion caused by the porous medium. The flux is then given by

$$\mathbf{q}_c = \phi c \mathbf{q} - \underline{\mathbf{D}} \cdot \nabla c \quad (5)$$

where c [kg m^{-3}] is the mass of species per unit volume of the fluid and $\underline{\mathbf{D}}$ is the dispersion tensor. As for the permeability, the dispersion tensor is symmetric. If it is assumed that the dispersion is horizontally isotropic, the principal directions are aligned with the Cartesian coordinate axes, and the dispersion varies only with depth, it takes the form:

$$\underline{\mathbf{D}} = \begin{bmatrix} D_H(z) & 0 & 0 \\ 0 & D_H(z) & 0 \\ 0 & 0 & D_V(z) \end{bmatrix} \quad (6)$$

The dispersion coefficients depend on fluid speed as well as the matrix geometry [see [Bear(1972)], and others, for a discussion]. The conservation equation, based on changes of solute mass per unit matrix volume, is:

$$\frac{\partial(\phi c)}{\partial t} = -\nabla \cdot \mathbf{q}_c - \phi \gamma c + \phi f(x, y, z, t) \quad (7)$$

where γ [s^{-1}] is the rate of removal of the species due to adsorption on the matrix surface or trapping in dead-end pores, and f [$\text{kg s}^{-1} \text{m}^{-3}$] is a source term (mass injection rate of species per unit volume of fluid). After substitution for \mathbf{q}_c , use of the above assumptions, and also that the components of $\underline{\mathbf{D}}$ are constant with depth, some rearrangement of (7) gives:

$$\frac{\partial c}{\partial t} = -\mathbf{q} \cdot \nabla c + D_H \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) + D_V \frac{\partial^2 c}{\partial z^2} - \gamma c + f \quad (8)$$

3 Homogeneous layer

For a single homogeneous confined layer of thickness H , with uniform flow u in the x -direction and constant dispersion coefficients, the species concentration after a uniform release Q [kg m^{-1}] from the line $(x, z) = (X, Z)$ at time $t = 0$, is given by:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D_H \frac{\partial^2 c}{\partial x^2} + D_V \frac{\partial^2 c}{\partial z^2} - \gamma c + Q \delta(x - X) \delta(z - Z) \delta(t) \quad (9)$$

with boundary and initial conditions:

$$\frac{\partial c}{\partial z}(0, t) = \frac{\partial c}{\partial z}(H, t) = 0$$

$$c(x, t) \rightarrow 0 \text{ as } x \rightarrow \pm\infty$$

$$c(x, 0^-) = 0 \quad (10)$$

corresponding, respectively, to zero flux through the bottom and top of the layer, vanishing concentration far away, and zero concentration before release. The zero flux conditions make the problem difficult to solve analytically, so a modelling device is used. The solution for an infinite system is known in terms of a Green's function. For Equation (9) with boundary and initial conditions:

$$c(x, t) \rightarrow 0 \text{ as } x, z \rightarrow \pm\infty$$

$$c(x, 0^-) = 0 \quad (11)$$

the solution is [see, for example, Kevorkian (1990)]:

$$c(x, t) = \frac{Q}{4\pi\sqrt{D_H D_V t}} \exp\left(-\frac{[x - (X + ut)]^2}{4D_H t} - \frac{(z - Z)^2}{4D_V t} - \gamma t\right) \quad (12)$$

An infinite set of image releases at points which are mirrored in the top and bottom surfaces are used, to ensure that the zero flux conditions apply at $z = 0, H$ (and in fact at all levels $z = nH, -\infty < n < \infty$). For the original problem (9) with (10), the solution is:

$$c(x, t) = \sum_{n=-\infty}^{\infty} \frac{Q}{4\pi\sqrt{D_H D_V t}} \exp\left(-\frac{[x - (X + ut)]^2}{4D_H t} - \frac{[z - (2nH + Z)]^2}{4D_V t} - \gamma t\right) \\ + \sum_{n=-\infty}^{\infty} \frac{Q}{4\pi\sqrt{D_H D_V t}} \exp\left(-\frac{[x - (X + ut)]^2}{4D_H t} - \frac{[z - (2nH - Z)]^2}{4D_V t} - \gamma t\right) \quad (13)$$

Figure 1 shows an example for a set of arbitrary, non-physical parameter values (for illustrative purposes only). In this computation, $-3 \leq n \leq 3$ is enough to get convergence.

4 Layered system

Conceptually, the non-homogeneous aquifer system is supposed to be composed of N (horizontal) layers with thicknesses d_k [m], porosities ϕ_k [-], fluid specific volume fluxes u_k [m s^{-1}], and horizontal dispersion coefficients D_k [$\text{m}^2 \text{s}^{-1}$], all for $k = 1, 2, \dots, N$. The fluid fluxes u_k are determined from the horizontal pressure gradient and layer permeabilities through Equation (3). At

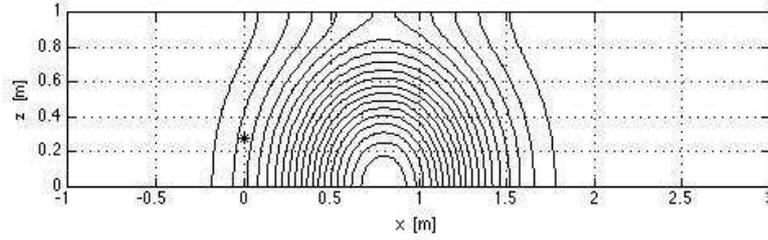


Figure 1: Concentration contours after $t = 0.8$ from a line release in a uniform layer with zero flux conditions at the top and bottom boundaries. The release line is marked *. Parameters are: $u = 1$, $D_H = D_V = 0.1$, $Q = 1$, $H = 1$, $Z = 0.275$, $\gamma = 0$ (all units given in the text).

the interfaces between the layers, it is supposed that there is a thin zone where mixing of the differently-concentrated layer fluids occurs, with transfer of pollutant from high to low concentration regions. The rate at which this occurs is quantified by interlayer transfer coefficients α_k [m s^{-1}], $k = 0, 1, 2, \dots, N$, that are assumed to be constants, but which are likely to depend on local flow shear, porosity contrasts, etc. The two-dimensional formulation described below may be readily generalized to include variation in the y -direction; however, the 2-D version allows easier conceptual clarity and graphical representation of solutions.

If $c_k(x, t)$ [kg m^{-3}] is the volumetric concentration of the pollutant in the fluid phase in Layer k , then over a small time interval $[t, t + \Delta t]$, within a small slice $[x, x + \Delta x]$ of Layer k , thickness d_k and (arbitrary but fixed) width W across the aquifer (within which the volume of fluid is $\phi_k W d_k \Delta x$), the net increase in mass of pollutant is given by the sum of the net influxes due to advection, dispersion, inter-layer transport, sources and sinks:

$$\begin{aligned}
 \phi_k W d_k \Delta x [c_k(x, t + \Delta t) - c_k(x, t)] = & W d_k u_k [c_k(x, t) - c_k(x + \Delta x, t)] \Delta t + \\
 & + \phi_k W d_k \left[-D_k \frac{\partial c_k}{\partial x}(x, t) + D_k \frac{\partial c_k}{\partial x}(x + \Delta x, t) \right] \Delta t + \\
 & + W \Delta x \alpha_{k-1} [c_{k-1}(x, t) - c_k(x, t)] \Delta t - \\
 & - W \Delta x \alpha_k [c_k(x, t) - c_{k+1}(x, t)] \Delta t + \\
 & + \phi_k W d_k \Delta x f_k(x, t) \Delta t - \phi_k W d_k \Delta x \gamma_k c_k(x, t) \Delta t + \\
 & + O(\Delta x^2 \Delta t, \Delta x \Delta t^2)
 \end{aligned} \tag{14}$$

where $f_k(x, t)$ [$\text{kg m}^{-3} \text{s}^{-1}$] is a pollution source term (mass injection of pollutant species per unit volume of interstitial fluid in Layer k), that may be distributed spatially and/or in time, and γ_k is a mass removal rate corresponding to adsorption on the matrix surface or trapping in pores. The latter “trapping” parameters are assumed constant, although in calculations below will be taken to be negligible compared with other terms and be given the values $\gamma_k = 0$. The inter-layer transport of the pollutant is assumed to be proportional to the difference in concentrations in adjacent layers, with α_k [m s^{-1}] (similar to osmosis parameters) being the inter-layer transfer rate coefficient for the interface between Layer k and Layer $k+1$ at $z = z_k$ ($k = 1, \dots, N-1$), with $\alpha_0 = \alpha_N = 0$ to reflect the impermeability at the upper and lower boundaries. Dividing (14) by $\phi_k d_k W \Delta x \Delta t$, taking the limits as $\Delta x \rightarrow 0$, $\Delta t \rightarrow 0$, and rearranging gives:

$$\begin{aligned} \frac{\partial c_k}{\partial t} = & -\frac{u_k}{\phi_k} \frac{\partial c_k}{\partial x} + D_k \frac{\partial^2 c_k}{\partial x^2} + \\ & + \frac{\alpha_{k-1}}{\phi_k d_k} c_{k-1} - \left(\frac{\alpha_{k-1} + \alpha_k}{\phi_k d_k} + \gamma_k \right) c_k + \frac{\alpha_k}{\phi_k d_k} c_{k+1} + f_k(x, t) \end{aligned} \quad (15)$$

Here, $\alpha_0 = \alpha_N = 0$, but otherwise the values may be non-zero. A zero internal α_k indicates that there can be no exchange between Layers k and $k+1$. The system of N coupled pde's is subject to boundary and initial conditions:

$$c_k(x, t) \rightarrow 0 \text{ as } x \rightarrow \pm\infty, c_k(x, 0^-) = 0 \quad (16)$$

Taking the Fourier transform (FT) w.r.t. x :

$$c_k(x, t) \rightarrow \hat{c}_k(\omega, t) = \int_{-\infty}^{\infty} e^{-i\omega x} c_k(x, t) dx,$$

and treating the transform parameter ω as a constant, gives:

$$\frac{d\hat{c}_k}{dt} = \beta_k \hat{c}_{k-1} - \xi_k \hat{c}_k + \zeta_k \hat{c}_{k+1} + \hat{f}_k(\omega, t) \quad (17)$$

where $\hat{c}_k(\omega, 0) = 0$ and

$$\beta_1 = 0, \xi_1(\omega) = i\omega \frac{u_1}{\phi_1} + \omega^2 D_1 + \frac{\alpha_1}{\phi_1 d_1} + \gamma_1, \zeta_1 = \frac{\alpha_1}{\phi_1 d_1}, \quad (18)$$

$$\beta_k = \frac{\alpha_{k-1}}{\phi_k d_k}, \xi_k(\omega) = i\omega \frac{u_k}{\phi_k} + \omega^2 D_k + \frac{\alpha_{k-1} + \alpha_k}{\phi_k d_k} + \gamma_k, \zeta_k = \frac{\alpha_k}{\phi_k d_k}, k = 2, \dots, N-1, \quad (19)$$

and

$$\beta_N = \frac{\alpha_{N-1}}{\phi_N d_N}, \xi_N(\omega) = i\omega \frac{u_N}{\phi_N} + \omega^2 D_N + \frac{\alpha_{N-1}}{\phi_N d_N} + \gamma_N, \zeta_N = 0. \quad (20)$$

The system of the N first-order differential equations in time may be written in matrix form:

$$\frac{d\hat{\underline{c}}}{dt} = A(\omega)\hat{\underline{c}} + \hat{\underline{f}}(\omega, t), \text{ with } \hat{\underline{c}}(\omega, 0) = 0, \quad (21)$$

where $\hat{\underline{c}}(\omega, t)$ is an $N \times 1$ column vector with elements $\hat{c}_k(\omega, t)$, and $A(\omega)$ is an $N \times N$ tri-diagonal matrix whose diagonal elements are complex functions of the parameter ω , as given above. In general, A is not symmetric. If $A(\omega)$ has eigenvalues and corresponding normalized eigenvectors $\lambda_k(\omega)$, $\underline{\xi}_k(\omega)$, $k = 1, \dots, N$, then we may form the $N \times N$ matrix P that has the eigenvectors as columns:

$$P = [\underline{\xi}_1 \quad \underline{\xi}_2 \quad \underline{\xi}_3 \quad \dots \quad \underline{\xi}_N] = P(\omega) \quad (22)$$

A is diagonalizable, and

$$P^{-1}AP = \begin{bmatrix} \lambda_1 & 0 & 0 & \dots & 0 \\ 0 & \lambda_2 & 0 & & 0 \\ 0 & 0 & \lambda_3 & & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \lambda_N \end{bmatrix} \quad (23)$$

Write $\hat{\underline{Z}} = P^{-1}\hat{\underline{c}}$. Then:

$$\frac{d\hat{\underline{Z}}}{dt} = P^{-1}AP\hat{\underline{Z}} + \hat{\underline{g}}(\omega, t), \text{ with } \hat{\underline{Z}}(\omega, 0) = 0 \quad (24)$$

where $\hat{\underline{g}} = P^{-1}\hat{\underline{f}}$. In terms of individual components:

$$\frac{d\hat{Z}_k}{dt} = \lambda_k \hat{Z}_k + \hat{g}_k(\omega, t), \text{ with } \hat{Z}_k(\omega, 0) = 0. \quad (25)$$

Solving, we find:

$$\hat{Z}_k(\omega, t) = \int_0^t e^{\lambda_k(t-\tau)} \hat{g}_k(\omega, \tau) d\tau \quad (26)$$

and $\hat{\underline{c}} = P\hat{\underline{Z}}$. Then, inverting the FT,

$$\underline{c}(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} \hat{\underline{c}}(\omega, t) d\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} P \hat{\underline{Z}}(\omega, t) d\omega \quad (27)$$

or, component-wise:

$$\begin{aligned} c_k(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} \sum_{j=1}^N P_{kj}(\omega) \hat{Z}_j(\omega, t) d\omega \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} \sum_{j=1}^N P_{kj}(\omega) \left(\int_0^t e^{\lambda_j t - \tau} \hat{g}_j(\omega, \tau) d\tau \right) d\omega \end{aligned} \quad (28)$$

The solutions are then found by quadratures. Certain simple forms for the initial source terms allows explicit integration with respect to time, and consequent fast computation of the concentration profiles. Some examples are given below.

5 Example calculations

5.1 Homogeneous layer with vertical dispersion

A simple test of the model is provided by a homogeneous layer with vertical dispersion, as already discussed in Section 3 above. When modelled by a multi-layered analogue, the inter-layer transfer parameters may be written in terms of an equivalent vertical dispersion parameter D_V . The vertical mass flux of pollutant per unit area across the interface between Layers k and $k + 1$, at $z = z_k$, is

$$-\alpha_k [c_{k+1}(x) - c_k(x)] \approx -D_V \left[\frac{\partial c}{\partial z} \right]_{z=z_k} \quad (29)$$

If the layers are thin, the vertical concentration gradient may be approximated reasonably well by

$$\left[\frac{\partial c}{\partial z} \right]_{z=z_k} = \frac{c_{k+1} - c_k}{\frac{1}{2}(d_k + d_{k+1})} \quad (30)$$

and the approximate equivalent value of α_k is then given by

$$\alpha_k \approx \frac{2D_V}{d_k + d_{k+1}} \quad (31)$$

If the single layer is subdivided into N layers of equal thickness $d = H/N$, the transfer coefficients are

$$\alpha_k \approx \frac{D_V}{d}, \quad k = 1, 2, \dots, N - 1. \quad (32)$$

By this means, vertical dispersion can be quantified using a multi-layer model.

Figure 2 shows results obtained after a time $t = 0.8$, for a “vertical sheet” release within the layer that is nearest to the line at $(x, z) = (0, .275)$, for comparison with Figure 1, where the analytic solution for the single-layer model was used. The multilayer model was calculated for cases where $N = 20, 10$ and 5 , with the contour lines being smooth interpolations of the c_k values within each of the layers. For the 20- and 10-layer cases, the patterns were almost indistinguishable from Figure 1. Even with only 5 sublayers (release in Layer 2) shown in Figure 2, the results are close to that from the single-layer model.

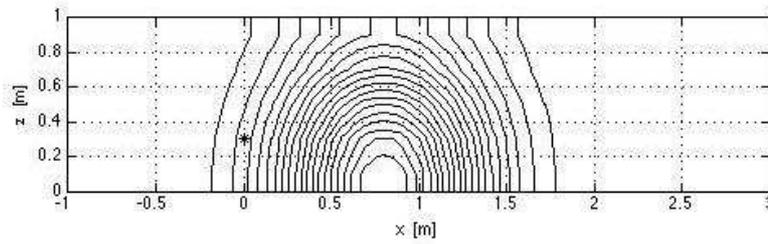


Figure 2: Concentration contours after $t = 0.8$ from a sheet release into Layer 2 of a multi-layered model with 5 layers. Other parameters are as in Figure 1.

5.2 Instantaneous areally-uniform source

Suppose a pollutant is released across all layers in a thin “sheet” perpendicular to the fluid flow. In that case, we may take $f_k(x, t) = q\delta(x)\delta(t)$, representing a uniform mass release q [kg m^{-2}] per unit aquifer cross-sectional area in all layers at $x = 0$, at time $t = 0$. Then $\hat{f}_k = q\delta(t)$, and

$$\hat{g}(\omega, t) = P^{-1}(\omega)\hat{f} = P^{-1}(\omega)\underline{L}q\delta(t) = \underline{G}\delta(t). \quad (33)$$

where \underline{L} is an $N \times 1$ column vector whose elements are all 1. The species concentration in each layer may be found by using:

$$\begin{aligned} c_k(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} \sum_{j=1}^N P_{kj}(\omega) \left(\int_0^t e^{\lambda_j(t-\tau)} G_j(\omega) \delta(\tau) d\tau \right) d\omega \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} \sum_{j=1}^N P_{kj}(\omega) e^{\lambda_j t} G_j(\omega) d\omega \end{aligned}$$

which gives a direct evaluation of the concentration at any given time $t > 0$ merely by performing a quadrature to perform the FT inversion (a FFT algorithm may be suitable).

5.3 Instantaneous uniformly-spread source

In the case where, at $t = 0$, the species is released uniformly within Layer k in the region $a_k \leq x \leq b_k$, the source function for that layer is

$$f_k(x, t) = \frac{Q_k}{d_k(b_k - a_k)} [\mathcal{H}(x - a_k) - \mathcal{H}(x - b_k)] \delta(t), \quad (34)$$

representing a mass release per unit aquifer width in the layer of Q_k [kg m⁻¹] spread uniformly over $a_k \leq x \leq b_k$, $z_{k-1} \leq z \leq z_k$. Then:

$$\hat{f}_k(\omega, t) = \frac{Q_k}{d_k(b_k - a_k)} \frac{i}{\omega} (e^{-ib_k\omega} - e^{-ia_k\omega}) \delta(t) = \hat{F}_k(\omega) \delta(t) \quad (35)$$

and

$$\hat{g}(\omega, t) = P^{-1}(\omega) \hat{f}_k(\omega, t) = P^{-1}(\omega) \underline{F}(\omega) \delta(t) = \underline{G}(\omega) \delta(t). \quad (36)$$

Then, as previously,

$$\begin{aligned} c_k(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} \sum_{j=1}^N P_{kj}(\omega) \left(\int_0^t e^{\lambda_j(t-\tau)} G_j(\omega) \delta(\tau) d\tau \right) d\omega \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega x} \sum_{j=1}^N P_{kj}(\omega) e^{\lambda_j t} G_j(\omega) d\omega \end{aligned} \quad (37)$$

Space allows only one example; that chosen is for three layers of equal thickness. The layer and release data are shown in Table 1. These are for illustration only and are deliberately chosen not to represent real data. Pollutant is released at $t = 0$ as a distributed source within each layer over various spatial intervals, and the “snapshot” in Figure 3 shows the concentrations at time $t = 2000$ s.

The initial release regions within each layer are delineated by dashed lines, while the concentrations at $t = 2000$ are shown by continuous lines. The effect of different flow speeds within the layers is seen, as are the changes in concentration in each layer due to that/those in adjacent layers. Because the process is dispersive, the concentrations become smaller as time proceeds.

Table 1: Parameters for example of spatial releases in the three-layer system.

Layer k	1	2	3
d_k [m]	1.0	1.0	1.0
ϕ [-]	0.1	0.2	0.1
u_k [m s ⁻¹]	50×10^{-6}	400×10^{-6}	100×10^{-6}
D_k [m ² s ⁻¹]	1×10^{-6}	1×10^{-6}	1×10^{-6}
γ_k [s ⁻¹]	0	0	0
α_k [m s ⁻¹]	1×10^{-3}	1×10^{-3}	-
Q_k [kg m ⁻¹]	0.2	1	0.4
a_k [m]	0	1	.4
b_k [m]	0.2	2	.8

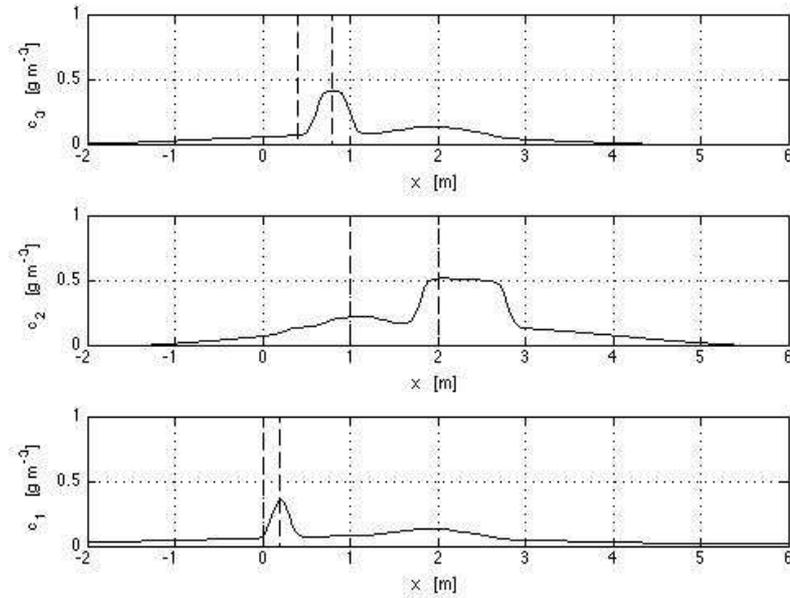


Figure 3: Concentration profiles in three adjacent layers a short time after extended spatial releases (between the dashed lines) in each layer. See Table 1 for parameters.

6 Summary

This paper describes some simple mathematical models that can be used to compute the dispersion of chemical species as they are advected by a fluid

flowing within a permeable matrix. The groundwater systems have (near-horizontal) layered structures and the linear advection-dispersion equations that model the transport have coefficients that depend mainly on depth.

The parameters that contribute to the coefficients in the partial differential equations are assumed constant within each layer, but can be different in each of the various layers. Anisotropy in permeability and in the dispersive length scales, as well as removal of the chemical by adsorption onto the matrix surface and movement into and/or out of dead-end pores, were all included. The resulting linear constant-coefficient pde's are coupled by mass flux continuity requirements at the layer interfaces. Full or partial analytic solutions for the species concentration were found, by using integral transforms, Green's functions and other techniques, thereby saving computational effort.

The modelling device of images was used to provide an analytical solution for species released into a homogeneous layer. For a multi-layered system, Fourier transforms allowed conversion to a dynamical system that was partly solved analytically using standard techniques. The layered system was also used as an approximate realization of an aquifer with properties that vary smoothly with depth. Space allowed only a small sample of examples. However, the computational algorithms for the general case may be readily deduced from the formulae given.

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