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Removing the boundaries to efficient groundwater contaminant transport modelling

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Abstract A solute transport modelling technique based on Markov process theory is developed. Transport is quantified by summing the first two moments of independent random displacements and applying the central limit theorem (CLT) to obtain the distribution of contaminant. For non-uniform flow fields the CLT is applied in a streamfunction/equi-travel time space, and transforms are used to give concentrations in Cartesian coordinates. Example simulations in a radially converging flow field show the method to be two to three orders of magnitude faster than modelling with the advection–dispersion equation; this is because the technique avoids the need to specify boundary conditions and solve linear algebraic equations.

INTRODUCTION

When a contaminant is released into a groundwater aquifer it may be considered to be transported by random movements, which give rise to a mean displacement and dispersion. To model this phenomenon it is common to apply numerical solutions to the advection–dispersion equation (ADE). Being a second-order differential equation, solution to the ADE requires specification of boundary conditions around the whole domain. However, when modelling most contaminant plumes, particularly in unconsolidated aquifers, it is usual to set the boundary concentrations to zero, or find that they evaluate to zero, when second or third type boundary conditions are specified. Are, then, the boundary conditions at all necessary?

While the boundary conditions are indeed a mathematical requirement for solving the ADE, they are not a physical requirement for contaminant transport. Solute movement in the plume occurs due to variations in velocity and to molecular diffusion; it is not affected by the contaminant concentration at a point tens or hundreds of metres down gradient.

The point of this observation is that solution of the ADE with its boundary conditions is computationally inefficient, requiring the formation and solution of linear algebraic equations. However, contaminant transport is essentially an additive random process and so could be modelled by much more efficient methods.

The objective of this work is to develop an efficient numerical *transport* modelling technique which does not require specification of boundary conditions and solution of linear algebraic equations. (Boundary conditions may still be required to solve the groundwater *flow* equation.) In fact, at least one such method already exists—the random walk approach. However, this is perhaps just as inefficient as solutions to the ADE by finite element or finite difference methods, since it involves random simulation. The method developed here is in the same spirit as the random walk approach, only it does not use random simulation, but solves for concentrations exactly by use of the central limit theorem (CLT).

The new modelling technique is developed by recognizing that the ADE, with a constant dispersion coefficient, is mathematically equivalent to a Markov process. Hence, the advection–dispersion phenomenon can be replicated by the summation of independent random displacements over incremental time steps. The actual distribution functions for displacements are unknown. However, after a sufficiently long flow time, they may be assumed to sum to a normal distribution by virtue of the CLT. Such an assumption is also inherent in the ADE, with the *a priori* use of Fickian dispersion.

The improved approach may be called the Sum of Moments Method. The first moment of the displacement is given by summing mean displacements in individual time steps along a streamline. The variance of the contaminant distribution at the time of interest is given by summing the second moments of the displacement functions, which may be expressed in terms of dispersivity coefficients.

A difficult challenge in developing this technique is to describe the contaminant distribution in a general flow field, defined numerically, which may include converging, diverging or bending streamlines. To achieve this goal it is necessary to sum moments and apply the CLT in a streamfunction/equi-travel time space and then apply a transformation to obtain the contaminant concentration in Cartesian coordinates.

Modelling results are presented for conservative contaminant transport in a two-dimensional (2-D) converging flow field. Results of the Sum of Moments Method are compared with numerical results obtained by a control volume technique, and the increased efficiency of the new approach is discussed.

CONTAMINANT TRANSPORT AS A MARKOV PROCESS

In developing a more efficient modelling technique, it is useful to recognize the foundations of the transport equation in Markov process theory. By considering the displacement of contaminant particles in a flow regime to be a Markov process, the ADE can be derived without the *a priori* assumption of Fickian dispersion

Following an instantaneous release of contaminant particles, the distribution of particle displacements $w(x_2[t_2])$ at time t_2 may be determined in terms of the distribution $w(x_1[t_1])$ at a previous time t_1 via the Smoluchowski or Chapman-Kolmogorov equation (Stratonovich, 1963):

$$w(x_2[t_2]) = \int p_{t_1,t_2}(x_1, x_2)\, w(x_1[t_1])\,\mathrm{d}x_1 \qquad t_2 > t_1 \tag{1}$$

In equation (1), p_{t_1,t_2} is a transition probability which characterizes variations in local flow velocity.

By expressing the transition probability in terms of its characteristic function equation (1) can be converted into a partial differential equation known as the Stochastic equation (Stratonovich, 1963):

$$\dot{w}(x) = \sum_{s=1}^{\infty} \frac{1}{s!}\left(-\frac{\partial}{\partial x}\right)^{s} \left[K_s(x)w(x)\right] \tag{2}$$

where the intensity coefficients, $K_s(x)$, are given by the moments $m_s(x)$, of p_{t_1,t_2} :

$$K_s(x) = \lim_{\tau \to 0} \frac{m_s(x)}{\tau} \tag{3}$$

Neglecting terms above second order, equation (2) reduces to the Fokker-Planck equation, which is identical to the ADE in its interpretation (Hathhorn, 1995):

$$\frac{\partial w}{\partial t} = -\frac{\partial}{\partial x}\left[K_1(x)w(x)\right] + \frac{\partial^2}{\partial x^2}\left[\frac{K_2(x)}{2}w(x)\right] \tag{4}$$

The parameters K_1 and $K_2/2$ are thus equivalent to the mean velocity and the dispersion coefficient.

It is important to note that equation (1) is simply the operation of summing together two independent random variables, and this process will be the basis of the new modelling technique.

It is interesting to observe how the requirement of boundary conditions is introduced in moving from the summation operation (1) to the ADE (equation (4)). In equation (1) the displacement distribution functions and the transition function are fully defined. However, by applying the Fourier transform and discarding terms above second order, indeterminacy is introduced. This indeterminacy is only overcome by constraining the distribution with boundary conditions. No boundary conditions are required for the system expressed by equation (1).

The process of discarding higher order terms in equation (2) is approximately valid by virtue of the central limit theorem. Since repeated application of operation (1) is equivalent to the repeated summation of independent random variables, the particle distribution that results from an instantaneous slug input would tend towards a Gaussian distribution as time increases. The Gaussian distribution is further recognized as being a fundamental solution to the ADE. In practice, contaminant distribution is not perfectly Gaussian and significant tailing effects can occur; this may be accounted for by the higher order terms in equation (2) (Kennedy & Lennox, 1999).

TRANSPORT MODELLING USING THE SUM OF MOMENTS METHOD

A numerical modelling technique based directly on Markov process theory can be developed using similar input requirements as when modelling by the ADE. Following discretization of the spatial domain and solution of the groundwater flow field, components of flow velocity and dispersion coefficients are defined for each cell or control volume. The coordinates of the contaminant source and time of release are also specified. Provided that the whole contaminant plume remains within the domain, boundary conditions are irrelevant.

Consideration will only be given here to an instantaneous point source. The contaminant distribution for a continuous or areal source can be subsequently determined using the principle of superposition.

Transport of the slug of contaminant may be considered to be a series of independent random particle displacements each occurring in a time step Δt_n. To obtain the displacement of the pollutant at some required time $T = \sum \Delta t_n$ the random movements are added together over incremental time steps.

Only the first two moments are required in the addition. Assuming the number of random movements, N, is sufficiently large, the distribution of the contaminant is Gaussian due to the CLT.

The distance between the point of injection and the centre of mass, μ_ψ, is given by the sum of the mean displacements $(\mu_\psi)_n$ during each time step:

$$\mu_\Psi = \sum_{n=1}^{N} (\mu_\Psi)_n = \sum_{n=1}^{N} (v(s))_n \Delta t_n \tag{5}$$

where $(v(s))_n$ is the velocity along the streamline during the nth time step Δt_n.

The second moments of contaminant spreading are also summed. So at time T, the variance in the direction of i (along the streamline or perpendicular to it) is:

$$\sigma_i^2 = \sum_{n=1}^{N} (\sigma_i^2)_n = \sum_{n=1}^{N} 2(D_i)_n \Delta t_n \tag{6}$$

where σ_i^2 and D_i are the variance and dispersion coefficient in the i-direction respectively.

APPLICATION TO NON-UNIFORM FLOW FIELDS

The method described so far is the essence of a modelling technique based on Markov process theory. The method is almost trivial when applied to a uniform flow field—the mean displacement and variances obtained from equations (5) and (6) fully determine the contaminant distribution. However, to be at all useful the technique must be able to describe the contaminant distribution in a general flow field, defined numerically, which may include converging, diverging or bending streamlines.

Under a non-uniform flow field the distribution of contaminant is clearly not Gaussian with respect to Cartesian coordinates. However, the CLT may still be applicable in a transformed frame of reference. Given sufficient flow time it may be assumed that the solute particles are normally distributed with respect to the solvent particles—only the latter have undergone net movement relative to each other.

Ericsson (1998) has developed a transformation from curvilinear coordinates to Cartesian coordinates that allows the CLT to be exploited. The contaminant is assumed to be normally distributed in a streamfunction/equi-travel time space, then the transform is used to obtain concentrations at locations defined in Cartesian coordinates.

In the case of a two-dimensional flow field, with mechanical dispersion dominating molecular diffusion, the distribution of contaminant in x, y coordinates with origin at the centre of mass is given by:

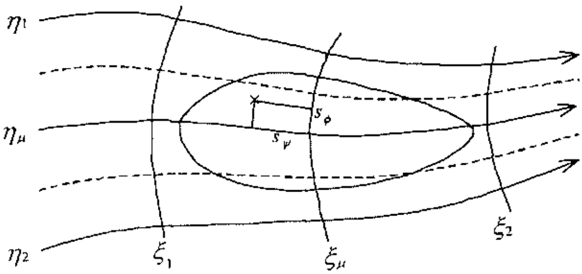

Fig. 1 Solute assumed to be normally distributed in transformed coordinates ξ, η.

$$w(x,y) = \frac{1}{2\pi\sigma_\xi\sigma_\eta} e^{-\frac{1}{2}\left[\frac{(\xi(s_\psi))^2}{\sigma_\xi^2}+\frac{(\eta(s_\phi))^2}{\sigma_\eta^2}\right]} \tag{7}$$

where $\xi(s_\psi)$ and $\eta(s_\phi)$ are potential and stream function values defined by distances s_ψ and s_ϕ in the transformed space (Fig. 1). The longitudinal and transverse variances, σ_ξ^2 and σ_η^2, in the transformed space are calculated from the usual longitudinal and transverse dispersivities, α_L and α_T, via:

$$\sigma_\eta^2 = 2\alpha_T\left(\mu_\Psi - s_\Psi^0\right) \tag{8}$$

$$\sigma_\xi^2 = 2\alpha_L v_\mu^2 \int_{s_\Psi^0}^{\mu_\Psi} \frac{1}{v_\Psi^2} \mathrm{d}s_\Psi \tag{9}$$

Numerically, σ_ξ^2 is calculated from the sum of the inverse squared velocity terms for each cell along the streamline from the source, s_ψ^0, to the centre of mass, μ_ψ.

The accuracy and efficiency of the Sum of Moments Method (SOMM) has been examined by modelling the transport of a conservative solute slug in a radially converging flow field. Results are compared with solutions obtained using a control volume modelling (CVM) technique (Kennedy & Lennox, 1995). Figure 2 shows the solute distribution for a quasi two-dimensional case considering longitudinal

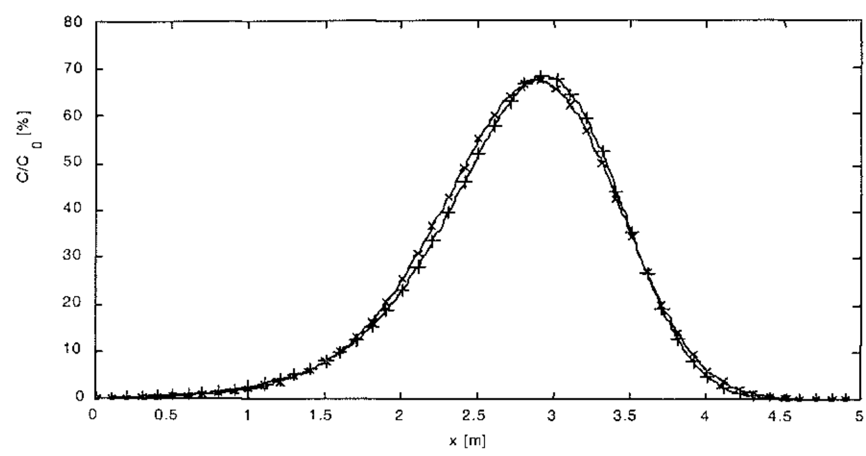

Fig. 2 Simulation of longitudinal transport in a converging flow field. Injection at $x = 4$ m with flow in the negative x direction. (-x-x-) = CVM; (-+-+-) = SOMM.

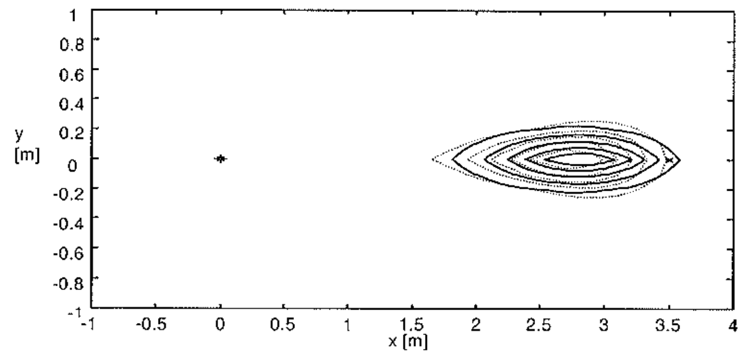

Fig. 3 Simulation of tracer transport in a radially converging flow field. Injection at x = 3.5 m, y = 0 m; pumping well at origin. (——) = CVM; (······) = SOMM.

dispersion only. Figure 3 compares contaminant contours for the full two-dimensional case. While there are slight discrepancies between the results from the two modelling techniques, the overall agreement verifies the SOMM.

To compare the efficiency of the two methods, both techniques were programmed using MATLAB and reasonable convergence to solutions was undertaken. For the quasi two-dimensional case the SOMM method was 2500 times faster than the CVM approach. For the two-dimensional case the difference was a factor of 300.

CONCLUSIONS

Contaminant transport can be modelled as a Markov process by a method that is two to three orders of magnitude more efficient than using the advection–dispersion equation. The method recognizes that contaminant transport theory is fundamentally underpinned by the CLT, and so it avoids the necessity of specifying boundary conditions and solving linear algebraic equations. The need to specify boundary conditions for the ADE follows from the indeterminacy that is introduced in truncating the stochastic equation (2) at second order.

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