A formula for predicting advection-dispersion in the vadose zone at uneven drainage intervals

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Abstract. A computational method is presented for predicting one-dimensional advective-dispersive solute transport with linear equilibrium sorption, for complex solute input histories associated with uneven intervals of transporting water flux. The suggested application is monitoring of leached solutes from land use and near-surface transformations, which are assumed to be transported through the vadose zone to the underlying groundwater without further degradation. Real-time forecasts of solute concentration at the groundwater surface provide a smooth feedback signal to operational management of land use for protection of groundwater, as a surrogate for groundwater monitoring which has unacceptable transport lag. The conceptual basis is the series of mixing cells as an analogue for advection-dispersion, in the form of a linear system for which cumulative pore-water drainage is the continuous index. This mixing-cell formula is unconditionally stable for any interval of drainage and assures conservation of solute mass. A demonstration example is presented.

1. Introduction

When land use is considered as a nonpoint source of groundwater contamination, the effects may be estimated, for the purposes of operational management, by assuming that solute which has been transported beyond transformation in the near-surface zone eventually reaches groundwater without further degradation. Examples of this kind of solute behavior are some pesticides and their degradation products, which have been leached below the organic layers of the soil, and nitrate anions leached beyond the influence of the plant root zone. The subsequent transport of these contaminants through the unsaturated vadose zone to the groundwater surface may be considered as an advective-dispersive process, which attenuates peaks in solute concentration but otherwise conserves solute mass. This process description can also include linear equilibrium sorption (onto solid surfaces or into immobile water) by appropriate scaling of the "water content" parameter with a "retardation" coefficient.

Leaching of contaminants below the near-surface zone is climatically driven, and inputs of contaminants to the vadose zone may be considered as intermittent amounts of drainage from the soil profile, each associated with a mass of contaminant in solution or suspension. The transport time to the groundwater surface may be several years, depending on depth to groundwater and geological properties. More significantly, the transport process is driven by the vertical water flux in the vadose zone, and transport time is therefore the cumulative effect of a series of drainage amounts generated by climate and soil-plant properties. Thus vadose zone transport is a stochastic process in terms of time, but in this note it will be presented as a deterministic process in terms of cumulative drainage.

The aim of this note is to provide a method for estimating the solute flux entering the groundwater surface in response to each drainage amount and associated contaminant concentra-

tion generated from beneath the soil layer. The purpose of this computation is to be able to forecast, in real time, the ultimate effect on groundwater quality of nonpoint source contamination generated by land uses such as land treatment of waste or application of fertilizers and pesticides for agricultural production. Where leachate quality and quantity are monitored, or estimated from a mathematical model, these data together with the vadose zone transport computation can provide a feedback signal for operational management of land use to achieve groundwater protection.

2. Transfer Function Approach

One-dimensional solute transport through the unsaturated subsurface zone can be represented in terms of a transfer function [*Jury*, 1982] which specifies the distribution of passage times to a particular depth. This concept is the same as the transfer function of a linear system, which can be defined as the output response to a unit input impulse. The time index can be replaced by cumulative drainage I for field-scale representation of solute transport under transient water flow [*Jury et al.*, 1990]. Numerical solutions [*Wierenga*, 1977] show that this transformation allows unsteady advective-dispersive solute transport to be adequately represented by the steady state solution. This characteristic depends on the dispersion coefficient D being linearly related to pore-water velocity V by a value of dispersivity λ which is invariant with water content. The water content θ for use with the steady state solution is suggested [*Wierenga*, 1977] to be near the value for field capacity. Other numerical results [*De Smedt and Wierenga*, 1978] support the use of a depth-averaged value of θ for nonuniform water content.

The time-based transfer function $f(t, L)$, at depth L, for advection-dispersion in soil under steady flow conditions, is [*Jury and Roth*, 1990, example 2.2]

$$f(t, L) = \frac{L}{t\sqrt{4\pi Dt}} \exp\left[-\frac{(L - Vt)^2}{4Dt}\right]. \qquad (1)$$

As a probability density function (pdf) of travel time t, (1) has mean L/V and variance $2DL/V^3$. The pdf $f(t, L)$ can be transformed to a cumulative drainage basis $f(I, L)$ by means of the equivalence $f(t, L)dt = f(I, L)dI$, substituting $D = \lambda V$, and then replacing the travel distance Vt with I/θ so that

$$f(I, L) = \frac{L}{I\sqrt{4\pi\lambda I/\theta}} \exp\left[-\frac{(L - I/\theta)^2}{4\lambda I/\theta} \right]. \quad (2)$$

The pdf (2) has mean $L\theta$ and variance $2L\lambda\theta^2$ and represents the transfer function of solute transported by advection with hydrodynamic dispersion. Therefore dispersion is assumed to be determined by the distance I/θ traveled by the cumulative water flux and is independent of the transient flow behavior.

The transfer function (2) completely characterizes advective-dispersive solute transport, but it is not a convenient mathematical form for prediction, especially for complex solute input histories and uneven intervals of drainage. The next section describes an analogous linear system which is more convenient for computational purposes.

3. Mixing-Cells Analogue

Solute transport through a series of cells, within each of which perfect mixing occurs, is a concept with a long history of dispersion modeling in hydrology [e.g., *Bear*, 1969; *Bajracharya and Barry*, 1994]. This model is often presented as an approximation to the finite difference solution of the advection-dispersion equation, and development has focused on problems of numerical dispersion and stability related to the size of the space and time steps [*Bajracharya and Barry*, 1992]. In contrast to these discrete-time models, series of mixing cells can also be described in continuous time by systems of ordinary differential equations which include solute transformations lumped at the scale of each cell [*Sardin et al.*, 1991]. The mixing cell volumes are predetermined so that their dynamic response simulates advective-dispersive transport, and the set of coupled differential equations for transport and transformation are solved by standard methods for complex linear systems [e.g., *Bidwell*, 1999].

Much of the mathematics of mixing-cell systems has emerged from chemical engineering and the theory of chromatography. *Van der Molen* [1956] applied the chromatographic theory of *Glueckauf* [1949], which includes linear equilibrium sorption, to leaching of saline soils. He describes the transport process in terms of soil-water flow (I), applies the principle of superposition of analytical solutions for complex salinity profiles, and estimates the parameter "theoretical plate thickness" from measurements of chloride ion concentration. This approach has essentially the same theoretical basis as (2), and the theoretical plate thickness is equivalent to 2λ. In a subsequent monograph [*van der Molen*, 1973] this dimension is called "effective mixing length," and the soil profile is considered as a series of mixing reservoirs for which the dynamic response is shown to simulate closely the analytical solutions from *Glueckauf* [1949]. This comparison is achieved by implicitly equating the time basis t and residence time T of a mixing reservoir to the flow basis I and the water content $2\lambda\theta$, respectively, of a theoretical plate. This equivalence is the same as that between (1) and (2).

A computational method is also provided for calculating the solute concentration $c_r(t)$ in cell r at time t, given the initial concentration $c(0)$ in each of the cells and input flux concentration c_{in} to the first cell. This procedure can be developed from the general solution of the ordinary differential equation of r mixing cells in series, each cell with residence time T. The general form of *van der Molen* [1973, equation (35)] is then

$$c_r(t) = c_{in} + [c(0) - c_{in}]\exp\left(\frac{-t}{T}\right)\left[1 + \sum_{m=0}^{r-1}\left(\frac{t^m}{m!T^m}\right)\right]. \quad (3)$$

For nonuniform initial concentration profiles, defined by $c_r(0)$, the principle of superposition leads to sequential application of (3) to the series of cells for computation of the concentration profile $c_r(t)$ at time t, which can be illustrated for the first three cells as

$$c_1(t) = c_{in} + [c_1(0) - c_{in}]\exp\left(\frac{-t}{T}\right)$$

$$c_2(t) = c_{in} + [c_1(0) - c_{in}]\exp\left(\frac{-t}{T}\right)\left(1 + \frac{t}{T}\right)$$

$$+ [c_2(0) - c_1(0)]\exp\left(\frac{-t}{T}\right)$$

$$c_3(t) = c_{in} + [c_1(0) - c_{in}]\exp\left(\frac{-t}{T}\right)\left(1 + \frac{t}{T} + \frac{t^2}{2!T^2}\right)$$

$$+ [c_2(0) - c_1(0)]\exp\left(\frac{-t}{T}\right)\left(1 + \frac{t}{T}\right)$$

$$+ [c_3(0) - c_2(0)]\exp\left(\frac{-t}{T}\right). \quad (4)$$

The general form of (4) can be rearranged as

$$c_r(t) = \exp\left(\frac{-t}{T}\right)\left[\sum_{m=0}^{r-1}\left(\frac{t^m}{m!T^m}c_{r-m}(0)\right)\right]$$

$$+ \left\{1 - \exp\left(\frac{-t}{T}\right)\left[\sum_{m=0}^{r-1}\left(\frac{t^m}{m!T^m}\right)\right]\right\}c_{in}. \quad (5)$$

These general solutions (3), (4), and (5) incorporate the implicit assumption that the input flux concentration c_{in} is constant over the time interval $\{0\ t\}$.

Bidwell [1999] developed a form of the mixing cell model, with flow basis I, which incorporates linear, equilibrium and nonequilibrium, solute transformation. For linear equilibrium processes, each cell has a resident volume per unit cross section [L] equal to $2\lambda\theta R$ (instead of residence time T), where the retardation coefficient R is the ratio of total mass to dissolved mass on a soil volume basis. This is the same as the *van der Molen* [1973] model if the process involves only equilibrium transfer of solute within the water phase, for which $R = 1$. For sorption onto solid surfaces, for which $R > 1$, the product $R\theta$ can be considered as a single parameter for calibration purposes if θ and R are not known independently. Solute mass balance of a cell is described by a differential equation with cumulative drainage I as the continuous index (instead of time t):

$$2\lambda\theta R\frac{dc}{dI} + c = c_{in}, \quad (6)$$

where c_{in} is the influent solute concentration. A series of n cells, each described by (6), is a linear dynamic system with a transfer function which is the gamma distribution

$$f(I, n) = \frac{I^{n-1}}{(n-1)!(2\lambda\theta R)^n} \exp\left[-\frac{I}{2\lambda\theta R}\right]. \quad (7)$$

The pdf (7) has mean $2n\lambda\theta R$ and variance $4n\lambda^2(\theta R)^2$. If the observation depth L is represented by n cells, then $L = 2n\lambda$, the mean is $L\theta R$, and variance is $2L\lambda(\theta R)^2$. The transfer functions of the advection-dispersion process (2) and the mixing-cell model (7) have the same mean and variance for $n = L/2\lambda$ and $R = 1$. The match between the two functions (2) and (7), over the full range of drainage I, improves with increasing number of cells and is very close for n greater than about 10.

4. Computational Form

For practical monitoring of leachate input to the vadose zone from land treatment of wastewater, for example, drainage collected from monolith soil lysimeters may be measured and sampled for bulk solute concentration at time intervals of about 1 month. The volume collected at the kth monitoring event is expressed as a drainage interval $dI(k)$, which depends on soil-water response to climate and irrigation events, and the corresponding bulk solute concentration $c_{in}(k)$ is considered to be constant during $dI(k)$. By substituting the following equivalences into (5)

$$c_r(k) \equiv c_r(t)$$

$$c_r(k-1) \equiv c_r(0)$$

$$c_{in}(k) \equiv c_{in} \quad (8)$$

$$dI(k) \equiv t$$

$$2\lambda\theta R \equiv T$$

and writing

$$\alpha(k) = \frac{dI(k)}{2\lambda\theta R}, \quad (9)$$

(5) then becomes

$$c_r(k) = \exp\left[-\alpha(k)\right]\left[\sum_{m=0}^{r-1}\left(\frac{\alpha(k)^m}{m!}c_{r-m}(k-1)\right)\right]$$

$$+ \left\{1 - \exp\left[-\alpha(k)\right]\left[\sum_{m=0}^{r-1}\left(\frac{\alpha(k)^m}{m!}\right)\right]\right\}c_{in}(k). \quad (10)$$

The formula (10) is unconditionally stable for any magnitude of drainage interval and assures conservation of solute mass. The number of mixing cells n required for a model is determined from the dispersivity λ and the depth L at which prediction is desired, according to

$$n = \frac{L}{2\lambda}. \quad (11)$$

The number of mixing cells n, from (11), may be large, for example, $n = 100$ for depth to groundwater $L = 20$ m and dispersivity $\lambda = 100$ mm. When the summation index m in (10) has these large values, evaluation of the ratio $\alpha(k)^m/m!$ by means of software library functions may cause numerical problems. These terms are better calculated by substituting
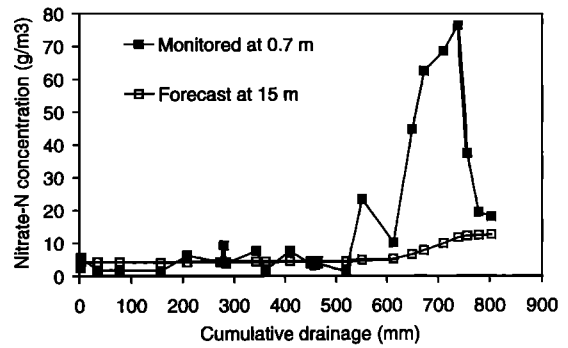
Figure 1. Forecasts of nitrate-N concentration at the groundwater surface (15 m depth), associated with monitored leachate concentrations from 0.7-m-deep lysimeters, as demonstrated for water content $\theta = 0.13$ and dispersivity $\lambda = 0.88$ m.

$$b_m(k) = \frac{\alpha(k)^m}{m!} \quad (12)$$

into (10) and calculating the coefficients $b_m(k)$ from the sequence

$$b_0(k) = 1$$

$$b_1(k) = \alpha(k)b_0(k)$$

$$\vdots \quad (13)$$

$$b_m(k) = \frac{\alpha(k)}{m}b_{m-1}(k)$$

$$\vdots$$

The value of the $b_m(k)$ coefficients may have very small values as m increases, depending on the value of $\alpha(k)$, and truncation of the process (13) may be considered. However, the author prefers to complete the full sequence and thus avoid having to test for loss of solute mass.

5. Demonstration Example

An example of the use of the computational method (9)–(13) is demonstrated with a series of flux-averaged nitrate-N concentration data $c_{in}(k)$ and average drainage fluxes $dI(k)$, collected from four monolith soil lysimeters used for monitoring a land treatment site for meat-processing wastewater [Bidwell, 2000]. These data were collected at approximately monthly time intervals during a 2-year trial for which the average drainage was 400 mm/yr. The data (Figure 1) include a significant "contamination event" when the waste treatment area was temporarily overloaded. The transport parameters θ and λ have not been determined for the vadose zone beneath the site, and for the purpose of the present demonstration, values have been used from measurements by Engesgaard et al. [1996] for the unsaturated zone of a sandy aquifer receiving estimated infiltration of about 450 mm/yr. Their results for fitting an advective-dispersive transport model to the tritium profile in the ~20-m-deep vadose zone provide values of $\theta = 0.13$ and $\lambda = 0.88$ m. For the present demonstration the depth to groundwater was set to 15 m.

It was assumed that for nitrate-N, $R = 1$, and there was no N transformation during advective-dispersive transport from

beneath the soil profile, at the 0.7-m monitoring depth of the lysimeter, down the remaining $L = 14.3$ m to the groundwater surface. The initial nitrate-N concentration in the vadose zone was set to the flux-averaged concentration for the first 12 months, of 4.4 g/m^3. For each input of drainage flux $dI(k)$ with average concentration $c_{in}(k)$, the concentration profile $c_r(k)$ was computed. Then a forecasted profile $c'_r(k)$ was obtained by applying an additional flux increment $dI'(k)$, at a concentration c'_{in} equal to the average solute concentration in the mixing cells, to transport $c_{in}(k)$ to the groundwater surface. In terms of (9) and (10) this computation is

$$dI'(k) = L\theta - dI(k)$$

$$c'_{in}(k) = \frac{1}{n} \sum_{r=1}^{n} c_r(k - 1)$$

$$\alpha'(k) = \frac{dI'(k)}{2\lambda\theta} \tag{14}$$

$$c'_r(k) = \exp\left[-\alpha'(k)\right] \left[\sum_{m=0}^{r-1} \left(\frac{\alpha'(k)^m}{m!} c_{r-m}(k) \right) \right]$$

$$+ \left\{ 1 - \exp\left[-\alpha'(k)\right] \left[\sum_{m=0}^{r-1} \left(\frac{\alpha'(k)^m}{m!} \right) \right] \right\} c'_{in}(k).$$

By means of (14), the estimated effect at groundwater level, $c'_n(k)$, can be computed on a real-time basis for each solute flux input monitored at the base of the surface soil. The computation takes into account advective-dispersive transport of the new input and the "background" concentration profile generated by the previous input history. Figure 1 shows the input data set and the corresponding forecasts at groundwater level for the parameters specified for the demonstration. These forecasted values can be used, in real time, as feedback information for operational management of the land treatment site. Groundwater level forecasts provide a more realistic signal than lysimeter data in terms of actual effect on groundwater, and the smoothing effect of the transport process improves the signal-to-noise ratio. Monitoring the actual groundwater contamination is not useful for operational management because of the long transport lag, which for the present demonstration is about 4.6 years.

6. Discussion

The methodology described in this note is for estimation of one-dimensional advective-dispersive transport in porous media, in response to complex data series of solute inputs at uneven intervals of transporting water flux. Dispersion is assumed to be linearly dependent on pore-water velocity but otherwise invariant with water content and is therefore completely described by the dispersivity λ. Linear equilibrium sorption processes can be included by means of a retardation coefficient R applied to the transporting water fraction θ or by calibration of the combined parameter θR. In conceptual terms, the mixing-cell analogue of advection-dispersion ac-

counts for resident solute concentration throughout the vadose zone depth. However, the parameters θR and λ are lumped values for the depth of observation, and the real distribution of concentration with depth may be different.

The computational procedure is intended for operational monitoring and management rather than as a conceptual model for scientific investigation and can support a range of feasible approaches to processing monitoring data. The example in this note demonstrates the use of forecasted contaminant effect at groundwater level for supporting operational management decisions, whereas the actual contaminant concentration in the groundwater may be the result of land-use events several years previous.

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