ground water

Discussion of Papers/ Christopher Neuzil, Discussion Editor

"A New Method for Laboratory Estimation of the Transverse Dispersion Coefficient" by M. Massabò, F. Catania, and O. Paladino, May–June issue 2007, v. 45, no. 3: 339–347.

Comment by Hund-Der Yeh[1] and Shaw-Yang Yang[2]

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Massabò et al. (2007) introduced a quick method for estimating the transverse dispersion coefficient in laboratory experiments without a priori knowledge of the longitudinal dispersion coefficient. The method is based on the analytical solution of the advective-dispersion equation (ADE) given in Massabò et al. (2006) for a pulse injection of a nonreactive solute in a soil column. They solved for the transverse dispersion coefficient as an unknown using an expression for the ratio of concentrations sampled at two points within the column. The exact solution for the concentration $C(r, z, t)$ is (Massabò et al. 2007, equation 5):

$$C(r,z,t) = \sum_{k=0}^{\infty} \frac{A_k}{\sqrt{4\pi t D_L}} \exp\left[-\frac{(z-ut)^2}{4D_L t}\right] \times \exp\left[-D_T \frac{Z_{k,1}^2}{R^2} t\right] J_0\left(Z_{k,1}\frac{r}{R}\right) \quad (1)$$

where D_L and D_T are the longitudinal and transverse dispersion coefficients, respectively, u is average linear velocity, r is radial distance from the centerline of the well, R is column radius, $J_0(\cdot)$ and $J_1(\cdot)$ are first kind Bessel functions of zero and first order, and $Z_{k,1}$ is the kth root of $J_1(\cdot)$.

The coefficient A_k in Equation 1 is defined as (Massabò et al. 2007, equation 7)

$$A_k = 2\frac{\sigma}{n}\frac{\rho}{R}\frac{J_1\left(\frac{\rho}{R}Z_{k,1}\right)}{Z_{k,1}[J_0(Z_{k,1})]^2} \quad \text{for} \quad k \neq 0$$
$$A_0 = \frac{\sigma}{n}\left(\frac{\rho}{R}\right)^2 \quad (2)$$

where σ is solute mass injected over the cross section, n is porosity, and ρ represents the radius of the injected solute. Massabò et al. (2007) mentioned that summing an infinite number of terms is required to obtain an accurate solution for the concentration $C(r, z, t)$ but, for practical applications, 1000 terms are sufficient.

In this comment, we suggest an alternative approach. The Shanks method (Shanks 1955) accelerates convergence when evaluating the Bessel functions and infinite series in Equation 1. The Shanks method is a nonlinear iterative algorithm based on the sequence of partial sums (Shanks 1955). This method has been successfully used in groundwater problems (see, e.g., Peng et al. 2002; Yeh et al. 2003). The Bessel functions in Equation 1 can be approximated by the formulas given in Watson (1958) and Abramowitz and Stegun (1964) and the large positive kth root, $Z_{k,v}$, can be approximated as (Yeh and Chang 2006):

$$Z_{k,v} = \beta - (4v^2-1)/(8\beta) - [4(4v^2-1)(28v^2-31)]/3(8\beta)^3 \quad (3)$$

where $\beta = (\pi/4)(2v + 4k - 1)$.

Let S_n represent a partial sum with n terms for an infinite series. A simplified expression for the Shanks transform developed by Wynn (1956) is:

$$e_{s+1}(S_n) = e_{s-1}(S_{n+1}) + \frac{1}{e_s(S_{n+1}) - e_s(S_n)}, \quad s = 1, 2, 3 \ldots \quad (4)$$

where $e_0(S_n) = S_n$ and $e_1(S_n) = [S_{n+1} - S_n]^{-1}$.

Applying the Shanks transform to compute a given series requires setting a convergence criterion defined as:

$$\left|\frac{e_{2r+2}(S_{n-1}) - e_{2r}(S_n)}{e_{2r+2}(S_{n-1})}\right| \leqslant \varepsilon \quad (5)$$

where ε is related to a desired accuracy. The running sum is terminated when this criterion is met.

Assume that $\sigma = 0.05$, $\rho = 0.05$ m, $n = 0.3$, $R = 0.1$ m, $r = 0.02$ m, $z = 1$ m, $u = 10^{-4}$ m/s, $D_T = 3 \times 10^{-9}$ m^2/s, and $D_L = 3 \times 10^{-1}$ m^2/s for $t = 3$, 30, or 300 s. Table 1 shows the numerical results for Equation 1 computed by the method we suggest here and the direct sum, which adds all the required terms until the specified accuracy criterion is met. The required terms for the direct sum with an accuracy to 10^{-7} are 888 and 86 when $t = 3$ and 300 s, respectively. For the same accuracy and test times, the suggested method requires fewer than 30

doi: 10.1111/j.1745-6584.2009.00618.x

Table 1
Required Terms in Achieving an Accuracy to 10^{-7} When Employing the Direct Sum and the Suggested Method to evaluate Equation 1 at Various Times

	Exact Solution	Number of Terms	
t (s)	$C(r, z, t)$	Direct Sum	Suggested Method
3	0.0375315	888	29
30	0.0152394	312	24
300	0.0049411	86	24

terms. Table 1 indicates that the number of terms for the direct sum with an accuracy to 10^{-7} increases significantly with decreasing time. Table 1 also indicates that the suggested method converges much faster than the direct sum when t is small. Obviously, the suggested method is computationally efficient for infinite series such as Equation 1. Moreover, it can also be used to compute the solution in terms of the unknown parameter, in this case the transverse dispersion coefficient (Massabò et al. 2007, equation 11).

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Note: Comment received August 26, 2007; accepted September 5, 2007.