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Comment on "An Analytical Solution for One-Dimensional Transport in Heterogeneous Porous Media" by S. R. Yates

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The solution to the deterministic one-dimensional advection-dispersion equation with distance-dependent dispersion coefficient derived by Yates [1990] has many advantages due to its analytical nature. The proposed model is interesting with potential practical applications in laboratory heterogeneous packed column solute transport experiments and possibly in some field studies where the assumption of one-dimensional flow under constant velocity is valid. The author should be commended for the useful analytical results presented. The objective of this comment is to report a simpler solution than the one given by Yates (1990) for the case of zero initial concentration and constant flux boundary condition. The notation employed here is identical to Yates (1990).

The correct general Laplace time solution to the governing advection-dispersion model is given by Yates [1990, equation (9)], assuming that the division of $\bar{C}(\xi, s)$ by C_0 on the left-hand side is in error. In order to satisfy the downstream boundary condition, the Laplace time solution reduces to

$$\bar{C}(\xi, s) = A(s) \xi^\gamma K_\gamma [2\gamma(s + \beta)^{1/2} \xi]. \quad (1)$$

The Laplace-transformed integration function, $A(s)$, is evaluated from the constant flux boundary condition [Yates, 1990, equation (15)]

$$-\frac{\xi_0}{2\gamma} \frac{d\bar{C}(\xi_0, s)}{d\xi} + \bar{C}(\xi_0, s) = \frac{C_0}{s}. \quad (2)$$

Substituting (1) into (2) and taking the derivative yields

$$A(s) = \frac{C_0}{s(s + \beta)^{1/2} \xi_0^{\gamma+1} K_{\gamma+1} [2\gamma(s + \beta)^{1/2} \xi_0]}, \quad (3)$$

where the following expression has been employed [McLachlan, 1955, p. 204; Gradshteyn and Ryzhik, 1980, p. 970]

$$z \frac{dK_\nu[z]}{dz} = \nu K_\nu[z] - z K_{\nu+1}[z]. \quad (4)$$

Substituting (3) into (1) leads to

$$\frac{\bar{C}(\xi, s)}{C_0} = \left[\frac{\xi}{\xi_0} \right]^\gamma \frac{K_\gamma [2\gamma(s + \beta)^{1/2} \xi]}{s(s + \beta)^{1/2} \xi_0 K_{\gamma+1} [2\gamma(s + \beta)^{1/2} \xi_0]}. \quad (5)$$

The preceding equation may be used as an approximate solution in conjunction with numerical inversion of the

Laplace transform by techniques such as the Stehfest algorithm [Stehfest, 1970], or Fourier series approximations [Dubner and Abate, 1968; Crump, 1976]. Yates [1990, equation (16)] is not in error, but (5) requires evaluation of only two modified Bessel functions and hence can be considered computationally less demanding. Following the procedure presented by Yates [1990, appendix], equation (5) is inverted from Laplace time variable s to real dimensionless time τ . The resulting solution is

$$\frac{C_r(\xi, \tau)}{C_0} = \left[\frac{\xi}{\xi_0} \right]^\gamma \left[\frac{K_\gamma [2\gamma\beta^{1/2}\xi]}{\beta^{1/2}\xi_0 K_{\gamma+1} [2\gamma\beta^{1/2}\xi_0]} \cdot \frac{2}{\pi} I_f \right], \quad (6)$$

where

$$I_f = \int_{\beta^{1/2}}^{\infty} \frac{\exp[-\chi^2\tau]}{\chi} \cdot \left[\frac{\phi(\chi) Y_\gamma(\epsilon) J_{\gamma+1}(\epsilon_0) - \phi(\chi) J_\gamma(\epsilon) Y_{\gamma+1}(\epsilon_0)}{\phi(\chi)^2 J_{\gamma+1}(\epsilon_0)^2 + \phi(\chi)^2 Y_{\gamma+1}(\epsilon_0)^2} \right] d\chi. \quad (7)$$

The solution (6) and (7) is more compact and easier to evaluate than that of Yates [1990, equations (17) and (18)]. It should also be noted that in (17) of Yates [1990] $\sqrt{\beta}$ should be replaced by $\sqrt{\beta}$.

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Reply

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Chrysikopoulos's [this issue] comment concerns the availability of a simpler form for the solution of the deterministic one-dimensional convective-dispersion with a distance-dependent dispersivity function for the case of an initial concentration of zero and a constant flux boundary condition.

The solution given by *Chrysikopoulos* is indeed a solution to equation (3) for the stated initial and boundary conditions. Since this solution requires the evaluation of four Bessel functions to obtain a value for the concentration at each location and time instead of six, it is a more efficient representation of the solution. Comparing the running time of identical programs which solve equation (17) of Yates [1990] and equation (6) of *Chrysikopoulos* [this issue] shows a reduction in computational time of about 30%, which can be attributed to the 1/3 reduction in the number Bessel functions that must be evaluated.

It should be pointed out, however, that both forms of the solution suffer from difficulties in numerical accuracy whenever the parameter γ gets large. For this situation, the ratio $(\xi/\xi_0)^\gamma$ and the Bessel functions in the range $0 < z < \infty$ can become very large, causing either numerical overflow or loss

of precision. Fortunately, as $\gamma \rightarrow \infty$, the solution to equation (3) of Yates [1990] approaches the classical convection-dispersion solution, where the dispersivity is constant. It is also possible to develop asymptotic solutions to this model for γ large. Two such solutions have been found and will be reported on in the future.

Chrysikopoulos's [this issue] remark that \sqrt{b} should be replaced with $\sqrt{\beta}$ is correct: a correction of this typographical error has been submitted.

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Correction to “An Analytical Solution for One-Dimensional Transport in Heterogeneous Porous Media” by S. R. Yates

In the paper “An Analytical Solution for One-Dimensional Transport in Heterogeneous Porous Media” by S. R. Yates (*Water Resources Research*, 26(10), 2331-2338, 1990) equations (9) and (17) contain a typographical error. These equations can be corrected by removing C_0 from the left-hand side of (9) and replacing \sqrt{b} multiplying the second term in the denominator of (17) with $\sqrt{\beta}$. I would like to thank C. V. Chrysikopoulos (1991) for pointing out these errors.

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