



Dispersion in VLEACH and Similar Models

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Abstract

VLEACH is a simple one-dimensional vadose zone leaching model capable of simulating volatile chemical transport. There is no explicit dispersion coefficient in VLEACH. Solutions computed with it show dispersion due to diffusion in the gaseous phase and its interaction with the liquid phase and also due to the discretization of the problem domain. By turning off gaseous diffusion and comparing VLEACH results to the standard convection dispersion equation, this Computer Note illustrates that the effective dispersivity due to the discretization is equal to half of the model cell size.

Introduction

VLEACH is a simple one-dimensional vadose zone leaching model that simulates volatile chemical transport (Rosenbloom et al. 1993; U.S. EPA 1996). As one of the individuals involved in the early development of VLEACH (along with Peter Lawson, Fritz Carlson, and primary author Jake Turin), I have found it rewarding to see its continued use and development. The recent release of a Windows version may make the program accessible to even more users. However, I was and continue to be concerned about the model's misapplication and misinterpretation of its output, particularly with respect to dispersion. Modelers, regulators, and other consumers of VLEACH results need to be aware of the significance of dispersion and its implicit nature in VLEACH and similar models. Dispersion is controlled by the model cell size.

VLEACH is fundamentally a mixing cell model in which mixing in every cell is instantaneous and complete at each time step (Bear 1972). VLEACH has no option for specification of dispersivity (α). Nevertheless, breakthrough curves generated with it—even when all explicit diffusive processes (diffusion in the gas phase) are turned off—clearly show dispersive behavior.

Impact of Dispersion

It should be well understood by modelers that the dispersivity, which is scale-dependent and notoriously difficult to estimate a pri-

ori, often has a pronounced effect on the concentrations computed at a receptor. In most VLEACH applications, the receptor is the water table. Gelhar et al. (1992) and Neuman (1995) have summarized dispersivity data from saturated zone solute transport measurements over a broad range of scales. These summaries indicate that, for a 10 m system for example, dispersivities range over three orders of magnitude from 10^{-2} to 10 m. Unsaturated systems may have an even broader range of dispersivities.

Figure 1 shows an example using an analytical solution of the Convection-Dispersion Equation (CDE) with four reasonable dispersivities for a nonretarded solute applied with the steady recharge water at a concentration of 100 mg/L to the top of a 10 m vadose zone for one year. The analytical solution was computed using CXTFIT (Toride et al. 1995) in flux concentration mode. Fortunately, the expected maximum concentrations at the water table vary far less than the three orders of magnitude variation in dispersivity, but they do vary by a potentially significant factor of four for the different dispersivities in this case. Relatively brief periods of high concentration in water supplies may be particularly problematic for at-risk consumers. Of course, in the absence of degradation or decay, mass balance dictates that all of the solute mass (provided loss of volatiles to the atmosphere is prohibited) will reach the water table eventually. Dispersion strongly affects the rate of loading to the water table, however.

Dispersion in VLEACH

The fundamental point I wish to make here is that, in VLEACH and any similar model, the dispersivity is implicit in the cell size (Δl) and equal to $\Delta l/2$ (Bear 1972). There seems to be no appreciation of this in the VLEACH developer and user communities. There are numerous applications of VLEACH where the cell size is simply based on collected data density, or worse, on arbitrary decisions by the modeler.

VLEACH solves a system of linear equations directly rather than using iterative methods. A Crank-Nicolson finite difference approximation is used to discretize the liquid advection process in VLEACH. Zheng and Bennett (1995) give the numerical dispersion associated with different discretization schemes.

Numerical modelers have repeatedly been cautioned (Anderson and Woessner 1992; Huyakorn and Pinder 1983) that they need to constrain their grid Peclet numbers so that $Pe = v\Delta l/D < 1$ to 10 (v is the mean pore water velocity and $D = \alpha v$ is the dispersion coefficient), but this is not pertinent here because D cannot be

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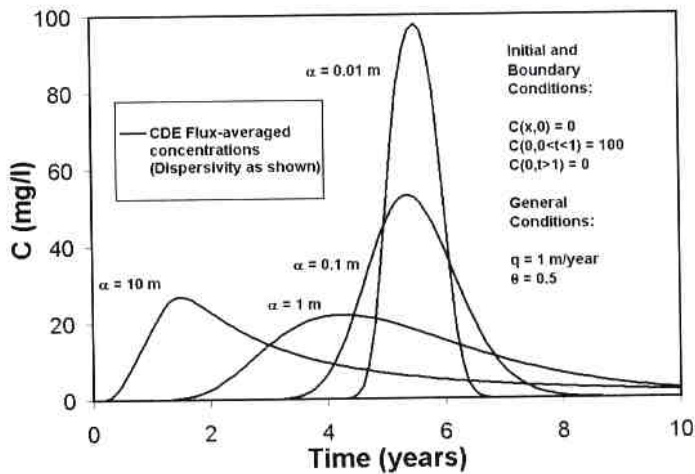


Figure 1. Flux concentrations at the base of a 10 m profile based on analytical solutions of the CDE for dispersivities in the range 10^{-2} to 10 m.

explicitly specified in the model. The time step, however, needs to meet the Courant number criterion ($Cr = v \Delta t / \Delta l \leq 1$) or instabilities arise.

Comparison of VLEACH and Convection-Dispersion Equation

Figure 2 compares analytical solutions of the CDE for three dispersivities with VLEACH solutions for three cell thicknesses. The initial condition of the model is uniform loading with a nonadsorbing, nonvolatile solute at 100 mg/L. At time 0, the model is flushed with solute-free water. Figure 2 shows close agreement between the VLEACH and analytical solutions for the 0.05 and 0.5 m dispersivities. The agreement is not as good for the 5 m dispersivity, which corresponds to only one 10 m thick cell in the VLEACH model, but the difference is usually relatively small. The VLEACH results for this case correspond exactly to the analytical solution $C/C_0 = e^{-(t/\tau)}$ for a mixing cell where τ is the residence time in the cell ($\Delta l/v$).

Conclusion

These results illustrate that dispersivity is implicit in VLEACH and is given by one-half of the cell size. Prudent selection of cell size will allow proper control of dispersion in the model. VLEACH users and those who interpret or make decisions based on VLEACH results need to be aware of this and of its impact on mass loading rates to ground water.

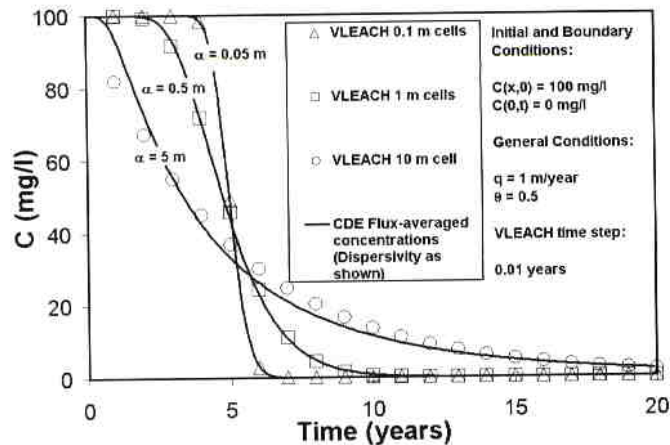


Figure 2. Concentrations at the base of a 10 m system independently simulated with the CDE (lines) and VLEACH (symbols). Dispersivities are explicitly specified in the CDE, but implicitly set by cell size in VLEACH.

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