KYSPILL: A Practical Modeling System of Scale-Dependent Dispersion after Chemical Spills

by Sergio E. Serrano[a]

Abstract

Scale-dependent dispersion is a phenomenon that manifests as an increase in the magnitude of the dispersion parameters with the distance of travel, or the time after the spill. This implies that contaminant plumes occupy a larger portion of the aquifer at later times than that predicted by the traditional convection-dispersion models. Although it is an area of active research, scale-dependent ground water pollution modeling is now available through the practical application of a new hydrologic theory of dispersion. The KYSPILL software was developed as an application of this theory. KYSPILL provides an easy way to simulate and graph the movement of contaminant plumes in heterogeneous soils and aquifers. It has self-supported menus and windows that allow the selection of the type of spill, the input of hydrogeologic data, and the plotting of contours and breakthrough curves. It simulates biological or radioactive decay, adsorption, point or nonpoint sources in the unsaturated zone and subsequently in the saturated zone. An automatic self-diagnosis system tests every input data, and an on-line, context-sensitive, help system aids the user in the input data and running phases. KYSPILL is a simple tool for those chemical spills with little or uncertain data. It may be used for preliminary forecasting, monitoring planning, or remedial actions.

Scale-Dependent Dispersion in Aquifers

The increase in the magnitude of the dispersion parameters with the scale of observation, or the time after a chemical spill, has been a problem of concern among hydrologists for the last two decades. In practical terms, this means that a contaminant plume will occupy a greater volume of the aquifer at later times than that predicted by traditional models based on the convection-dispersion equation (CDE). This phenomenon has been termed "scale-dependent" contaminant dispersion. Among the possible explanations for this are: (1) it has been reported that the Fickian approximation is strictly valid at small laboratory scales; (2) aquifer heterogeneity at field scales appears to play a major role in the enhanced value of the dispersion parameters; (3) the effect of seasonal variability in the recharge from rainfall; and (4) the presence of boundary conditions that determine the regional hydraulic gradients.

Many theories of scale-dependent dispersion phenomena remain at the level of theoretical scientific research. Some works conceive the growth in the dispersivity parameter as deterministic functions of distance or time (e.g., Pickens and Grisak 1981; Gupta and Bhatthacharya 1986; Barry and Sposito 1989; Yates 1990). Other works study the stochastic representation of the hydraulic conductivity in a heterogeneous aquifer (e.g., Bakr et al. 1978; Dagan 1984, 1986; Gelhar and Axness 1983; Neuman et al. 1987; Rubin 1991). In this paper we focus on the practical applications of a new hydrologic theory of dispersion (Serrano 1996, 1995a). This theory is based on the consideration of the aquifer's regional hydrology, as well as the aquifer heterogeneity at the field scale. It recognizes that the variability in the field flow velocity depends not only on the spatial variability of the hydraulic conductivity, but also on important hydrologic functions such as recharge from rainfall, the value of the boundary conditions, and their transient characteristics. After considering the statistical properties of the hydraulic conductivity and the functional form of hydrologic functions, the resulting differential equations are solved via the method of decomposition (Adomian 1994). Decomposition is a relatively unknown method, which allows a systematic analytical solution of complex linear and nonlinear, and deterministic or stochastic, equations.

As an application to the new hydrologic theory, the KYSPILL software (HydroScience Inc. 1996) was developed. KYSPILL is a user-friendly software program written in C that implements several of the new decomposition solutions and presents them in practical graphical form. It also incorporates the modeling of unsaturated zone plumes, adsorption, and decay, and couples these with subsequent plume propagation in the saturated zone. The result is a simple and flexible tool for preliminary simulation of contaminant plumes after chemical spills.

Modeling of Scale-Dependent Dispersion

As a brief overview of the essence of scale-dependent dispersion modeling, consider the simplest case of a solute transport equation with time-dependent dispersion coefficients in a two-dimensional aquifer with Dupuit assumptions:

$$\frac{\partial C}{\partial t} - \bar{D}_x(t)\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} - \bar{D}_y(t)\frac{\partial^2 C}{\partial y^2} = 0 \qquad (1)$$

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where C is the mean contaminant concentration (ML^{-3}); u is the mean pore velocity, predominantly in the x direction (LT^{-1}); and x and y represent longitudinal and transverse distance from the spill location, respectively (L); t is time after the spill (T); and $\bar{D}_x(t)$ and $\bar{D}_y(t)$ are the longitudinal and transverse dispersion coefficients, respectively (L^2T^{-1}). Equation 1 is subject to the boundary and initial conditions corresponding to the field situation and the spill class under consideration. One estimate of the field-scale dispersion coefficients is (Serrano 1996)

$$\bar{D}_x(t) = D_x + \sigma_u^2 t$$
$$\bar{D}_y(t) = D_y + \frac{c\sigma_u^2 t}{l^2} \quad (2)$$

where D_x is the small-scale longitudinal dispersion coefficient (L^2T^{-1}); D_y is the small-scale transverse dispersion coefficient (L^2T^{-1}); σ_u^2 is the variance of the pore velocity u $(LT^{-1})^2$, which is functionally dependent on the hydrology and hydraulics of the aquifer; l is the transmissivity correlation length (L); and c = 2.0 (L^2).

The application of Equation 2 requires estimates of the aquifer transmissivity at several locations in the aquifer. With as many point values of the transmissivity as possible, the hydrologist needs to estimate the statistical average of the transmissivity, $\bar{T}$, the transmissivity variance, σ_T^2, and the correlation length of the transmissivity, l, using the standard statistical formulae. The parameter l is a measure of correlation between individual values of transmissivity. For example, highly correlated transmissivity values (a homogeneous aquifer) reflect large values of l (i.e., 100 m). On the other hand, uncorrelated values of transmissivity (a heterogeneous aquifer) reflect low values of l (i.e., 10 m). Thus, while σ_T^2 represents the individual variability in T from point to point, l represents the degree of spatial association between individual values. Strictly speaking, this number should be estimated from a calculation of the serial correlation coefficient. However, the hydrologist rarely has sufficient information for such a test, and instead has to rely on a limited number of punctual values. Knowing that the accuracy of this estimate of the dispersion coefficient increases with the number of transmissivity samples, the hydrologist has to use common sense and experience in estimating statistical parameters.

The variance of the pore velocity, σ_u^2 is calculated from the aforementioned statistics of the transmissivity, and knowledge of the hydrologic conditions affecting the aquifer. For instance, for the classical unconfined aquifer bounded by two rivers of known head, the variance of the pore velocity is given by (Serrano 1995b)

$$\sigma_u^2 = \frac{\sigma_T^2 A^2}{n^2 h^2} \quad (3)$$

where n is the porosity; h is the hydraulic head with respect to the bottom of the aquifer (L); and A is a parameter depending on recharge and boundary conditions. See Serrano (1997) for numerical examples on the calculation of each parameter.

Equations 2 and 3 illustrate the principle that aquifer dispersion parameters are explicit functions of the aquifer hydrology, the statistical properties of the transmissivity (as a measure of aquifer heterogeneity), and the time after the spill. According to decomposition theory, the scale effect is the result of hydrologic field conditions (e.g., recharge from rainfall and flow boundary conditions), and aquifer heterogeneity at the field scale. The solute mass conservation equation is essentially valid at any scale. The Fickian approximation constitutes an initial condition to the evolution of the contaminant plume at large scales. Generalizations of this model to two-dimensional and three-dimensional domains (Serrano 1996), and verification with limited tracer tests, confirm this hypothesis. This concept is consistent with recent observations on the behavior of Fractal dynamical systems, where measures of system parameters repeat themselves and grow with the scale of observation. According to decomposition theory, this is reflected in the increase in magnitude of the variance of the output process and results solely from the initial condition input to a nonlinear dynamical system (Adomian 1994).

From Equation 2, the dispersion coefficients are not asymptotic functions of time, as the small perturbation theories propose. Instead, the dispersion coefficients keep evolving until the physical limits of the aquifer are found, in agreement with results elsewhere (Matheron and de Marsily 1980). The conceptual differences with the classical theories could be traced to the fundamental assumptions adopted by the different theories, and the mathematical methods of solution used. The classical theories neglect specific features of a given aquifer hydrology, use the logarithmic transformation of the hydraulic conductivity, and use the small perturbation approximation to the equations (e.g., Bakr et al. 1978; Dagan 1984, 1986; Gelhar and Axness 1983; Neuman et al. 1987; Rubin 1991). The decomposition theory considers the aquifer hydrology as well as the statistical properties of the aquifer transmissivity. It uses the "raw" field transmissivity, and approaches the true solution of the equation without restricting the size of the parameters. In summary, advection, molecular diffusion, and mechanical dispersion are the fundamental physical processes affecting hydrodynamic dispersion of conservative contaminants at small scales. Aquifer recharge, flow boundary conditions, and transmissivity spatial variability (i.e., heterogeneity) are the processes affecting dispersion at large scales.

The solution to Equation 1 subject to Equation 2 and a particular set of boundary and initial conditions is given in Serrano (1996, 1995a). The KYSPILL software implements these solutions and links them to solutions of transport equations in the unsaturated zone when the spill originated in the soil (or the vadose zone), rather than the aquifer. In such a case, the original point source for the unsaturated zone becomes a distributed source for the saturated zone once the contaminant has migrated to the interface with the water table.

Other scenarios implemented by the software include the case of biological or radioactive decay, adsorption, stationary sources (e.g., long-term leakage from an underground storage tank), and the case of nonpoint sources. Nonpoint sources occur when the initial spill (or the plume when the hydrologist first visits the site) occupies a large area. In such a case, the model is fed with a series of concentration values taken at individual sampling points, along with their coordinates with respect to a reference point (e.g., the center of the spill). KYSPILL will then implement a numerical algorithm to estimate the probable form of the original spill and will forecast its future movement.

Using KYSPILL for Practical Ground Water Pollution Modeling

As stated before, KYSPILL is a practical computer program created for the purpose of predicting scale-dependent contaminant

migration in random porous media. It incorporates several solutions of the dispersion equation with a user-friendly interface, an automatic data diagnosis, a set of self-supported menus, graphics, and windows, and a context-sensitive on-line help system. The model uses the solution of a differential equation that corresponds to the type of spill selected by the user (i.e., the initial condition) and plots the solution in a form selected by the user.

From a practical point of view, the hydrologist needs to select the type of contamination problem appropriate for the site. For that purpose, s/he will need to classify the spill according to its hydrologic zone location, its time regime, and the spatial distribution of its initial condition. First, the hydrologic zone location of the spill must be determined: unsaturated or saturated zone spill. This stems from an observation of the source and the plume at the time of the initial investigation. Sanitary landfill leachates and leaks from underground storage tanks are examples of unsaturated zone spills. Well releases are examples of saturated zone spills. Second, the time regime of the source is determined: short- or long-term spill. Sanitary leachates are examples of long-term, or stationary, spills. Accidental spills are examples of short-term, or transient, spills. Third, the spatial distribution of the initial condition is determined: point or nonpoint source. A spill from a truck is an example of a point source. A plume occupying a large portion of an aquifer is an example of a nonpoint source. An on-line help system aids the user in selecting the spill type from the menu according to the given field conditions.

The selected spill will open an input data screen, where hydrologic and hydrogeologic data of the spill area are entered, including precipitation and air temperature that the model uses to estimate recharge, partition coefficients, degradation rates for nonconservative contaminants, porosity, mean values of hydraulic conductivity and its standard deviation from the samples taken in the field, mean hydraulic gradient, and the fractions of clay and sand in the soil to estimate field capacity. In the case of nonpoint sources, the user may enter an array of individual concentration sample values and their coordinates with respect to a selected origin. Every data value entered is automatically screened for validity. There is also an on-line, context-sensitive help system that aids the user in estimating values of unavailable or inaccurate data.

When the data screen is closed, the user can choose a variety of graphics from a menu: surface or profile contours, time or space breakthrough curves, etc. The user may see the contours in the unsaturated zone at a specified time, or in the saturated zone once the contaminant propagates into the aquifer. Most simulation models of ground water pollution limit their attention to the solution of contaminant transport problems either in the unsaturated zone or the saturated zone. This is due in part to the conceptual difficulties in representing mass transfer at the interface between the unsaturated and saturated zones, and the mathematics of subsequent propagation in the saturated zone subject to a nonpoint source at the interface. Yet an accidental chemical spill at the ground surface, which slowly penetrates through the unsaturated zone and eventually propagates through the saturated zone, constitutes a frequent problem of practical importance. With KYSPILL, the simulation in the two zones is easily accomplished.

As an illustration on the effect of scale on the size of the plume, let us imagine that a certain amount of a contaminant was released through a well. We wish to forecast the contaminant concentration distribution in the future. The following parameters were measured: initial concentration, adjusted for the mass, is 500 mg/L; soil porosity is n= 0.1; aquifer mean hydraulic gradient is 0.001 m/m; small-scale aquifer longitudinal dispersivity is 1.0 m; small-scale aquifer transverse dispersivity is 0.1 m; retardation factor is 1.0; degradation constant is 0.0 month^{-1}; and aquifer mean hydraulic conductivity is $\bar{K}$= 100.0 m/month. For a scale-independent, or a homogeneous aquifer, problem we set the conductivity standard deviation σ_K = 0.0 m/month and "raw" conductivity correlation length l = 100.0 m. Figure 1 shows a cross section of the plume (i.e., C versus x) 120 months after release. Now, we re-run the program for a mildly heterogeneous aquifer (e.g., σ_K = 30.0 m/month). Figure 2 shows the same plume section for a scale-dependent condition. Note that the maximum concentration is about six times less for the scale-dependent plume than that of the scale-independent plume. However, the most important effect of scale is the enhanced area covered by the plume: in the x direction, the scale-independent plume extends from x = 70 m to about x = 170 m, as opposed to from x = −90 m to x = 250 m for the scale-dependent plume. This means that 10 years after release, the contaminated area is about three times greater than that predicted by small-scale calculations. This could have serious implications in environmental decisions.

As a second illustration, let us imagine that a small spill of a certain contaminant occurred at the ground surface and that the hydrologist has estimated the following parameters: initial con-

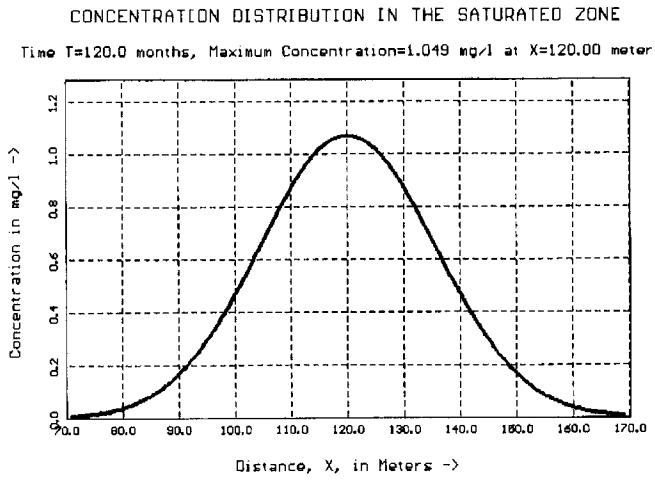

Figure 1.

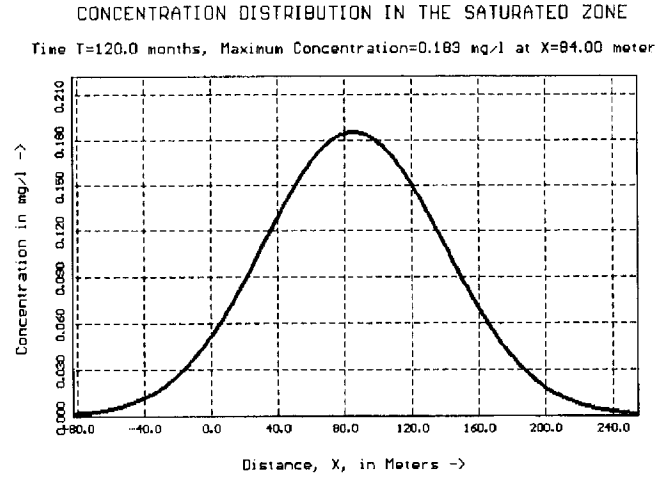

Figure 2.

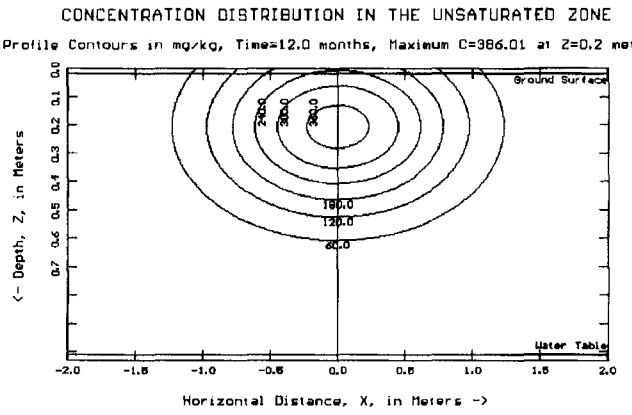

Figure 3.

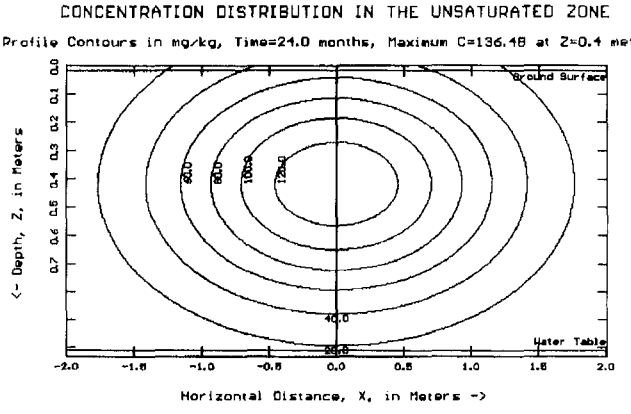

Figure 4.

centration adjusted for the mass is 500 mg/kg; small-scale soil horizontal dispersivity is 1.0 m; small-scale soil vertical dispersivity is 0.1 m; mean annual precipitation is 1000 mm/year; mean annual air temperature is 10°C; water table depth is w = 1.0 m; soil dry bulk density is γ_s = 1500 kg/m^3; soil composition is 75% sand and 5% clay. KYSPILL estimates a mean monthly recharge rate from a water balance that accounts for evapotranspiration and uses it as the mean vertical advection rate for the plume. In the unsaturated zone, a three-dimensional dispersion equation is solved. In this example, assume the same values of the previous example for the saturated zone.

Figures 3 and 4 show the unsaturated zone concentration contours 12 and 24 months after the spill, respectively. Figures 5 and 6 show the saturated zone plan view concentration contours 120 and 144 months after the spill, respectively. Note that due to the slow penetration of the source from the unsaturated zone, the saturated zone plume is not symmetrical with respect to the peak in the longitudinal direction. It is also interesting to observe that the maximum concentration remains somewhat close to the origin, and that only after a prolonged period of time, when most of the contaminant from the unsaturated zone has entered the saturated zone, will the plume tend to become symmetric.

KYSPILL may be run with little or preliminary data to assess the possible ("what if") contamination scenarios. It may help in the design of monitoring networks and function as a preview for more detailed numerical simulation models. However, for the average ground water pollution problem, where data is severely limited in quantity and quality, it may be the only viable and practical choice.

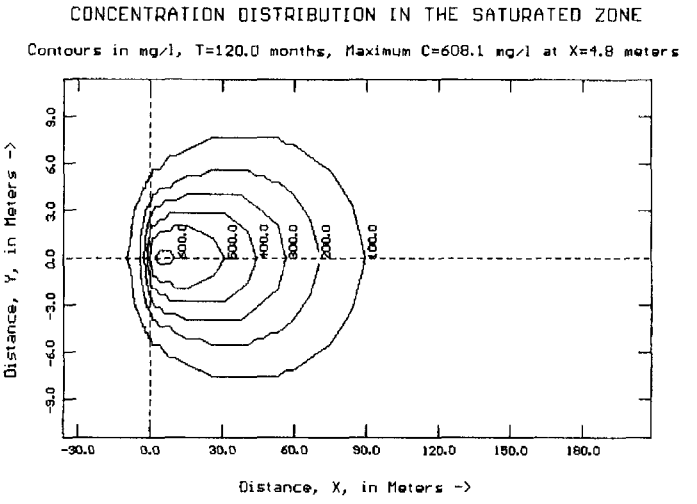

Figure 5.

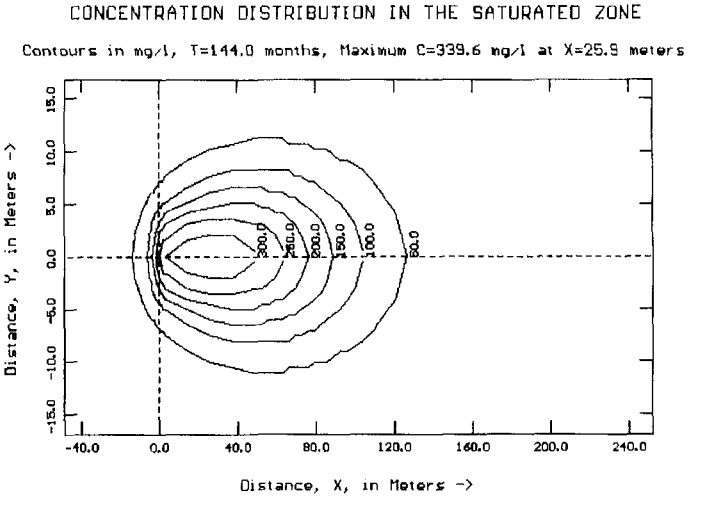

Figure 6.

KYSPILL Specifications and Availability

KYSPILL Version 2.1 (HydroScience Inc. 1996) is available in one 3.5-inch diskette and a user's manual. Version 2.1 contains six modules that handle point and nonpoint sources in the unsaturated and saturated zones, as well as stationary sources. KYSPILL Version 1.2 is also available as part of a new hydrology book (Serrano 1997) at a reduced price. Version 1.2 contains the two main modules for unsaturated zone and saturated zone spills. As of this writing, it is a DOS-based program for the IBM PC, although it may be run under Windows 3.1 or Windows 95. Minimum requirements are 640K RAM, a math co-processor, and VGA graphics card. It uses very little memory and may be run from a floppy disk driver, although a hard disk is highly desirable.

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