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UNCERTAINTY IN MODEL CALIBRATION AND VALIDATION FOR THE CONVECTION-DISPERSION PROCESS IN THE LAYERED VADOSE ZONE

R.J. Glass, T.S. Steenhuis, G.H. Oosting and J.-Y. Parlange

Department of Agricultural Engineering

Cornell University, Ithaca New York

ABSTRACT

The validation of models for contaminant transport in the vadose zone is a difficult task. In this paper we consider the application of the convection-dispersion model to describe the movement of a non-reacting, non-adsorbing, non-degradable solute through layered but otherwise homogeneous sand. An experimental data set is used to calibrate the model which is then used to predict the outcome of similar experiments. We conclude that goodness of fit in one case is no guarantee of success in another, if the model does not describe the physical processes with sufficient precision.

INTRODUCTION

To describe the transport of solutes through the unsaturated zone two main approaches, statistical and phenomenological, have been used and advocated by researchers. The statistical approach parameterizes the solute travel time structure from measured concentrations either in the laboratory or in the field without being overly concerned with the physics of the basic process (e.g., transfer function models for solute transport developed by Jury, (1982) and Jury et al., (1986)). The phenomenological approach conceptualizes the solute transport process as a deterministic mathematical model which is then solved using either analytical or numerical techniques (e.g., Parker and van Genuchten, (1984); Rao et al., (1980a,b)). A combination of the two approaches either in the form of a statistical selection of parameter values for the mathematical model or the incorporation of random variables themselves into the governing equations to form stochastic equations has been used to bridge the gap between theory and observation (e.g., Tang et al., (1982); Gelhar, (1986); Knighton and Wagenet, (1987)). Models which incorporate statistics are often data limited and thus are difficult to apply in the field because the input data are not generally available or too expensive to measure. Thus, deterministic modeling in the form of screening models (e.g., Steenhuis and Naylor, (1987); Jury et al., (1987)) is often used to assess the impact of land management practices such as pesticide application or waste repository siting on ground water quality.

Mathematical modeling of solute transport at the microscopic level (i.e., at an individual pore or pore sequence basis) is difficult because of the complex pora geometry of the soils. Hence, most mathematical models describe the solute transport at the macroscopic level (e.g., Rao et al., (1980a,b)). At the macroscopic level, chemicals are convected with the fluid and undergo a dispersion process which mixes or smears the chemical about the position of the average pore velocity. Superimposed upon this movement are chemically related processea such as adsorption-desorption, reaction and degradation. The convection-dispersion process has been extensively researched (see Bear, (1976)) and considered by many to be adequately understood. This confidence is reflected in the fact that deviations from prediction have been attributed to additional processes, often chemically related and not to the failure of the modeling of the bulk fluid flow and corresponding dispersion. Many management and research level computer models are based on the convection-dispersion model with various additional chemical processes, e.g., GLEAMS (Leonard et al., (1986)), PRZM (Carsel et al., (1985)), CMIS (Nofziger and Hornsby, (1986)), LEACHEM (Wagenet and Hudson, (1986)), and MOUSE (Steenhuis et al., (1987)). It is therefore extremely important to validate convection-dispersion theory for soils especially for soils typically overlying aquifers.

In this paper, we examine the use of the convection-dispersion equation for modeling the transport of solutes through the vadose zone. Here we are not concerned with the chemical processes and instead focus on the convection-dispersion process as it is important for modeling the transport of any chemical. Thus we consider the simplest of cases, the transport of a non-reacting, non-adsorbing, non-degradable solute through layered but otherwise homogeneous sand columns in the laboratory. The convective-dispersion model has long been assumed to be valid for this simple system and thus analytical solutions are available for homogeneous and layered soils (e.g., Barry and Parker, (1987)).

For the purpose of this examination, we will use the breakthrough curves presented in Class et al., (1988) for laboratory columns which simulate a soil profile much like that overlying major aquifers in post glaciated regions containing a fine-textured surface layer and a coarse sand

subsoil. In three of the experiments the flux through the system was approximately the same but were separated by a period of no inflow. In one experiment the flow rate was reduced. We investigate the ability of parameters obtained in one of the experiments to predict the solute transport observed in the other experiments, each with slightly different conditions.

We find that predictive capability is poor thus raising concerns about standard validation methodology and pointing out the severe difficulty faced by those who wish to accurately model solute transport in the layered vadose zone based on the convection-dispersion model.

MODELING AND MODEL VALIDATION METHODOLOGY

There are four main steps in the modeling process: mathematical formulation, solution generation, solution verification and model validation. The first step consists of a conceptualization of the physical system and the development of a comparable mathematical model that reflects the physical system.

The second step is the solution of the mathematical model using appropriate boundary and initial conditions. The solution may use analytical or numerical methods and often models are confusingly referred to as analytical or numerical models depending on their solution technique.

The third step is the verification that the solution of the mathematical model is correct and involves the checking for mathematical or programming errors. Verification of analytical solutions is easily accomplished by substitution back into the governing equations. Numerical solutions are best verified by comparison with particular analytical solutions. In the absence of any analytical solution for verification purposes, comparison between several different numerical solutions of the same mathematical model is a less desirable but unavoidable alternative.

The fourth step compares the solution of the mathematical model to the physical reality which it claims to describe and is correctly termed model validation. There is much debate about the question of when a model is considered validated and can be used "safely" for prediction. The definition used by the International Atomic Energy Agency states that (IAEA, 1982 quoted by Tsang, (1987)):

"A conceptual model and the computer code derived from it are validated when it is confirmed that the conceptual model and the computer code provide a good representation of the actual process occurring in the real system. Validation is thus carried out by comparison of calculations with field observations and experimental measurements".

The comparison is usually first attempted in a controlled laboratory experiment. A laboratory experiment is almost always a caricature of the natural system, hence, mathematical models that are to be applied in the field must also be validated there. For either laboratory or field validation, input parameters for the mathematical model must be appraised. Model parameters are either measured directly or estimated by applying the model to a controlled experiment and fitting the data to the model solution. The fitting process itself, whether done on an individual parameter such as the determination of hydraulic conductivity by applying Darcy's Law, or on all parameters simultaneously is nothing more than model calibration. In order to validate the model, parameters measured through calibration must then be used in the model to predict correctly the system response in experiments for which the model is not calibrated. It is often assumed that if the model can predict the system response in one or two different settings then the model is "validated" and can be used to predict the physical system response in a much wider range of circumstances. This assumption, however, can lead to serious error as we discuss later.

THE CONVECTION-DISPERSION MODEL

For one dimensional steady state water flow conditions and non-adsorbing, conservative solutes at concentrations, mass continuity for the solute may be written

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \qquad (1)$$

where C is the soil water solution concentration, D the dispersion coefficient, v the average pore water velocity, t the time and x the space coordinate.

In equation (1), two transport processes are incorporated. The first is convective transport given by the last term on the right hand side of equation (1) parameterized by the average pore water velocity, v. The pore velocity can be estimated by the quotient of the water flux and the average moisture content behind the wetting front. The second transport process is a solute mixing process termed dispersion given by the first term on the right hand side of equation (1) parameterized by the dispersion coefficient, D.

Equation (1) is the well known convective-dispersion equation which often is assumed to govern the transport of solutes through homogeneous porous media. The dispersion coefficient theoretically incorporates molecular diffusion, hydrodynamic dispersion and other mechanical mixing processes with the molecular diffusion significant only at low flow velocities (Bear, (1976)). Hydrodynamic dispersion is the macroscopic outcome of the

passive movement of solute particles by the highly variable velocity field within individual pores. It is a non-steady, irreversible process. Other mechanisms can cause mixing which may be lumped into the dispersion coefficient such as the effect of spatial variability in the transport properties of the porous medium itself or more specifically the effects of cracks and macropores.

While microscopic models have been proposed to predict dispersion, the empirical nature of macroscopic properties which average over many complicated interactions must be emphasized and the only realistic way to obtain an estimate of the dispersion coefficient D is through experimentation. Experiments are designed such that analytical solutions to the flow equations apply and the solution is fitted to the data. For instance, approximate solutions for solute transport in layered soil have been developed by Barry and Parker, (1987). They show that two layer systems may be approximated by an equivalent one layer (homogeneous) system, when the ratio of the equivalent single layer Péclet number, P_e, and the sum of the Péclet numbers of the individual layers, P_1 and P_2, is larger than 0.5, viz

$$\frac{P_e}{P_1 + P_2} > 0.5 \qquad (2)$$

The Péclet number is dimensionless and defined by the product of the average pore velocity and the length of the layer divided by the dispersion coefficient. For our two-layered experiments described in the following section, we meet the criteria as stated in (2) snd thus we may substitute an equivalent homogeneous one-layer system for our two-layer system. An analytical solution of equation (1) with flux averaged boundary conditions has been given by Parker and van Genuchten, (1984) and their program which optimizes parameters using a non-linear inversion method is used to fit our data to the model.

A common extension of the convection dispersion model that allows the fitting of many asymmetrical breakthrough curves is the two "zone" model, where "zone" can either be in the physical sense of mobile-immobile water or in the chemical sense of two-site adsorption-desorption (Rao et al., (1979)). For the two-zone model, convective and dispersive transport is restricted to the mobile water phase and transport into and out of the immobile water is diffusion limited. Equation (1) may be rewritten as (Parker and van Genuchten, (1984)):

$$\beta \frac{\partial C_1}{\partial t} + (1-\beta) \frac{\partial C_2}{\partial t} = D \frac{\partial^2 C_1}{\partial x^2} - v \frac{\partial C_1}{\partial x} \qquad (3)$$

$$(1-\beta) \frac{\partial C_2}{\partial t} = \omega \frac{v}{L} (C_1 - C_2) \qquad (4)$$

where β is the ratio of the mobile water content to the total water content
L the length of the column and

$$C_1 = \frac{C_m - C_i}{C_0 - C_i} \qquad (5)$$

$$C_2 = \frac{C_{im} - C_i}{C_0 - C_i} \qquad (6)$$

C_m mobile water concentration
C_i initial concentration of the solute in the column
C_0 concentration of the infiltrating water
C_{im} concentration of the immobile water and

$$\omega = \frac{\alpha L \theta_m}{v} \qquad (7)$$

where α is the first order rate constant that governs the rate of solute exchange between the mobile and immobile regions and θ_m is the mobile moisture content. An analytical solution to equations (3) and (4) for flux averaged boundary conditions given by Parker and van Genuchten, (1984) is also fitted to the data using their curve fitting program.

EXPERIMENTAL DESCRIPTION

The layered column consisted of a 129 cm high coarse bottom layer composed of US sieve series fraction 14-40 silica sand and an 8 cm high fine top layer of silica sand which passed a #200 sieve. The cross-sectional area of the chamber was 51 cm^2. The technique of Glass et al., (1988) was used to insure that the column was homogeneous within each layer so that complications of heterogeneity on the flow process could be minimized.

Two replicates (sets) of three consecutive infiltration experiments were conducted. A fourth infiltration experiment was not replicated. In each infiltration experiment pulses of USDA blue #1 dye solution (approximately 0.058%) were used to characterize the solute movement. Pulses were sdded by allowing the ponding level to decrease from 1.5 cm to 1 cm after which 25.5 ml of a known concentration of blue dyed water was mixed thoroughly in the ponded water. Constant ponding to a level of 1.5 cm was resumed just as all blue dyed water had moved into the top layer. The subscripted number in the experiment label refers to the blue pulse number.

In the first infiltration experiment, denoted by a capital "A" following the replicate number, the sand was initially air dried. A depth of 1.5 cm of water was ponded and maintained for 72 hours during which solute pulses were added at 4, 24 and 48 hours. The chamber was then sealed at the top to inhibit evaporation and allowed to drain by

gravity for twenty-four hours. The moisture content field at the end of the drainage cycle formed the initial moisture field for the second experiment.

The second infiltration experiment, denoted by a capital "B" following the replicate number, was then conducted with a steady ponding level of 1.5 cm for 72 hours again with solute pulses at 4, 24 and 48 hours. After 24 houra of drainage of this "B" experiment, 1.5 cm of water was added every 8 hours for a two week period with the first 1.5 cm containing the solute. This experiment, simulating intermittent irrigation events, we denote by "B_{int}" following the replicate number.

TABLE 1: Experiments Conducted

Experiment Run Number	Initial Moisture Condition	Flow Rate
		(ml/min)
$1A_1$	dry	21.74
$1A_2$		20.88
$1B_1$	1 day after 1A	19.98
$1B_2$		16.98
$1B_{int}$	1 day after 1B	0.14
$2A_1$	dry	21.35
$2A_2$		20.97
$2A_3$		20.05
$2B_1$	1 day after 2A	20.05
$2B_2$		20.74
$2B_3$		19.63
$2B_{int}$	1 day after 2B	0.14
$2C_1$	1 day after $2B_{int}$	20.00
$2C_2$		18.66
$2C_3$		19.22

In preparation for the fourth and final experiment, the bottom layer was saturated several times, sealed and drained for another twenty-four hours. A uniform moisture content of about 6% in the bottom layer resulted. This final experiment was also conducted with a steady ponding level of 1.5 cm for 72 hours with solute pulses at 4, 24 and 48 hours and is further denoted by a capital "C" following the replicate number. In this way the first ("A") and fourth ("C") experiments represented the initial moisture content conditions (i.e., uniform) often used in analytical and numerical studies of infiltration flows. The second and third experiments mimic more realistically field situations where initial moisture content is that left by the previous infiltration event, and infiltration is either steady ("B") or intermittent ("B_{int}"). Table 1 presents a summary of all the experiments conducted.

As can be seen in Table 1 the flux through each of the columns in the "A", "B" and "C" experiments was approximately 0.4 cm/min while for the experiment where the water was applied intermittently the average flux was 0.16 cm/hr.

RESULTS

The figures presented hereafter show the results of the various calibration (or parameter fitting) and validation scenarios detailed in Teble 2. The valuea of the parameters used are contained in Table 3. A total of 4 validation scenarios were constructed from the data set, however many more could have been examined. Parker and van Genuchton's, (1984) parameter fitting program fits any combination of D and v to the solution of equation (1). For the solution of equations (3) and (4), the two-zone model, the additional paramoters β and ω may be fitted. Since the flux through the system varied slightly between the "A", "B" and "C" experiments and v is given by the ratio of the flux and the average moisture content, we chose initially in each scenario to assume that the average moisture content was the same and thus modified v by the flux that occurred.

Figures 1a, 1b, 1c and 2 relate to the "A" experiments in which the water infiltrated into the initially dry sand. Figure 1a shows the data points for $2A_1$ and the fitted solution to equation (1). In Figure 1b, the observed outflow concentrations of the second and third breakthrough

TABLE 2: Validation Scenarios

Scenario	Description
1	Use optimized D and θ values for first breakthrough curve $2A_1$ to predict the second and third breakthrough curve $2A_2$ and $2A_3$ within the same replicate and experiment.
2	Use average optimized D and θ values for experiment 2A where water infiltrated in the dry soil to predict outflow concentration for the replicate also in dry soil 1A.
3	Use average optimized D and θ values for experiment 2A where water infiltrated in the dry soil to predict outflow concentration for next experiment 2B after one day with no water addition.
4	Use average optimized D and θ values of steady state experiments 2A and 2B to predict the concentration in experiment $2B_{int}$ where water was applied intermittently.

curves of the second replicate ($2A_2$ & $2A_3$) are compared with the predicted outflow concentrations using input data (dispersion and average moisture content) for the solution shown in Figure 1a. The flux from each experiment was used with the average moisture content from $2A_1$ to calculate v. Although the agreement between predicted and observed outflow concentrations is satisfactory, the tail is not predicted well in either Figure 1a or 1b. To investigate whether the two-region model would give a better prediction for the observations near the tail, we used the second breakthrough curve for replicate 2 ($2A_2$) as a test. Figure 1c shows that the two-region model does not improve greatly the prediction of the outflow solute concentration over that for equation (1). The tail is predicted a bit better, but at the expense of the other parameters.

To demonstrate the ability of fitted experimental values to carry over from one experiment to an identical experiment (scenario 2), in Figure 2 the average fitted dispersion coefficient and moisture content of the three breakthrough curves of replicate 2 are used to predict the two breakthrough curves for the first replicate. (Solid line is the prediction based on replicate 2 values). The velocity of the water was again obtained by dividing observed flux by the average moisture content from replicate 2. The agreement is close and at least as good as the prediction based on fitted parameters for each experiment itself (broken lines).

Next we use the parameters (dispersion and moisture content) obtained from the A experiment to predict solute movement in the B experiment (scenario 3). This is shown in Figure 3a. A very poor prediction indeed! Due to the shift in the

TABLE 3: Origin and Value of Parameters

Figure[a]	Dispersion Coefficient D (cm^2/min)		Moisture Content θ (cm^3/cm^3)		Water Flux (mm/min)		Pulse Time Solute App. (min)		Mobile/ Immobile β		Exchange Rate ω		OBSERVED DATA PLOTTED	Symbol in Figure
1a	$2A_1$[b]	8.40	$2A_1$	0.078	$2A_2$	4.39	$2A_1$	1.99	-	-	-	-	$2A_2$	+
1b (1)	$2A_1$	8.40	$2A_1$	0.078	$2A_2$	4.11	$2A_1$	1.99	-	-	-	-	$2A_2$	X
	$2A_1$	8.40	$2A_1$	0.078	$2A_3$	3.93	$2A_1$	1.99	-	-	-	-	$2A_3$	0
1c (1)	$2A_2$	8.40	$2A_2$	0.079	$2A_2$	4.11	$2A_2$	1.99	-	-	-	-	$2A_2$	*
	$2A_2$	0.28	$2A_2$	0.079	$2A_2$	4.11	$2A_2$	1.99	est	0.5	$2A_2$	22.1		
2 (2)	$2A_{av}$	8.26	$2A_{av}$	0.080	$1A_{av}$	4.18	$1A_{av}$	1.56	-	-	-	-	$1A_1$	+
	$1A_1$	11.78	$1A_1$	0.085	$1A_1$	4.26	$1A_1$	1.51	-	-	-	-	$1A_2$	•
	$1A_2$	13.09	$1A_2$	0.090	$1A_2$	4.10	$1A_2$	1.61	-	-	-	-		
3a (3)	$2A_{av}$	8.26	$2A_{av}$	0.080	$2B_{av}$	4.12	$2B_{av}$	2.10	-	-	-	-	$2B_1$	+
	$1A_{av}$	13.56	$1A_{av}$	0.080	$2B_{av}$	4.12	$2B_{av}$	2.10	-	-	-	-	$2B_2$	*
													$2B_1$	o
3b (3)	$2A_{av}$[c]	4.86	$2B_{av}$	0.137	$2B_{av}$	4.12	$2B_{av}$	2.10	-	-	-	-	$2B_1$	+
	$2B_2$	16.40	$2B_2$	0.137	$2B_2$	4.12	$2B_2$	2.33	-	-	-	-	$2B_2$	*
													$2B_3$	o
4a (4)	$2A_{av}$[c]	0.10	$2A_{av}$[d]	0.046	$2B_{int}$	0.027		• 260	-	-	-	-	$2B_{int}$	x
	$2B_{av}$[c]	0.07	$2B_{av}$[d]	0.103	$2B_{int}$	0.027		• 260	-	-	-	-		
4b (4)	$2B_{int}$	0.48	$2B_{int}$	0.071	$2B_{int}$	0.027	$2B_{int}$	243	-	-	-	-	$2B_{int}$	x
	$2B_{int}$	0.60	$2B_{int}$	0.084	$2B_{int}$	0.027	[f]	324	$2B_{int}$	0.89	$2B_{int}$	13.8		

[a] See Table 2 for definition of the scenarios given in parentheses.
[b] Letter and number combination refers to experiments described in Table 1. Values in column that follows are based on the particular experiment.
[c] Dispersion adjusted for observed fluxes.
[d] Moisture content adjusted for fluxes.
• Calculated to force 25% of mass left in column (as observed).
[f] Calculated to force conservation of mass.

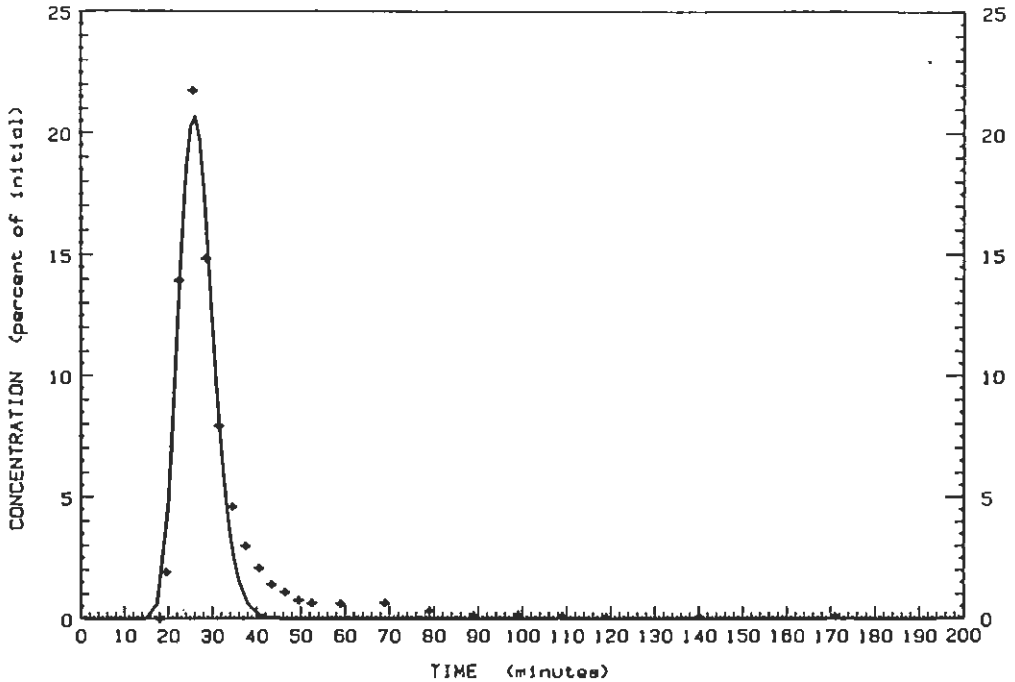

Figure 1a. Breakthrough curve for experiment $2A_1$ (+). Solid line shows the fitted solution to equation 1.

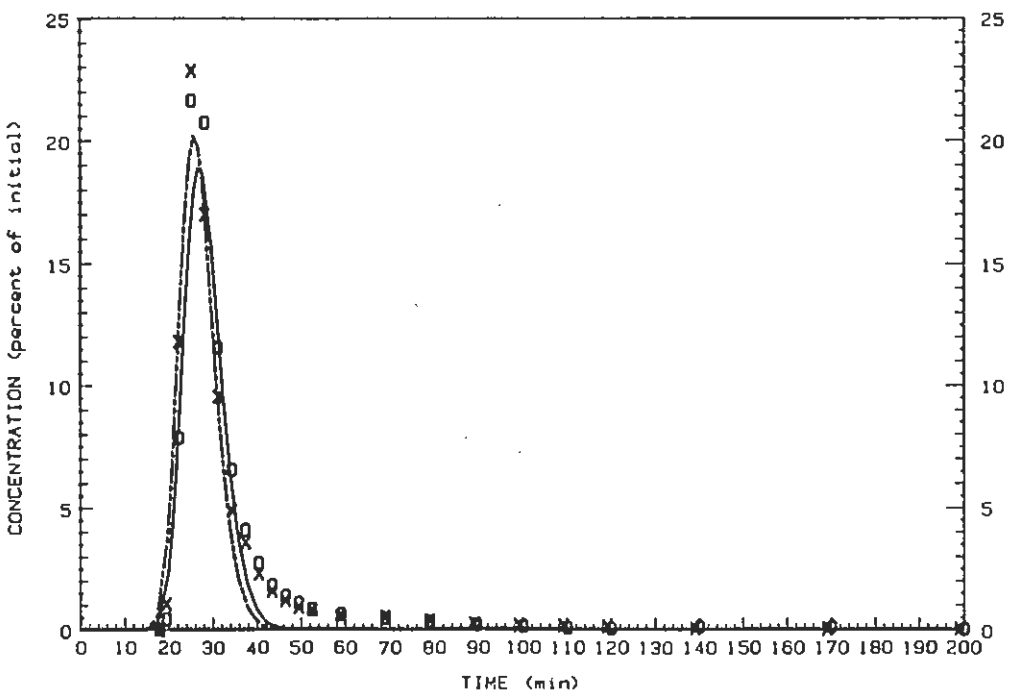

Figure 1b. Scenario 1, breakthrough curves for experiment $2A_2$ (x) and $2A_3$ (o). Solid and broken lines are predicted for $2A_2$ and $2A3_1$ respectively with the fitted D and θ from experiment $2A_1$.

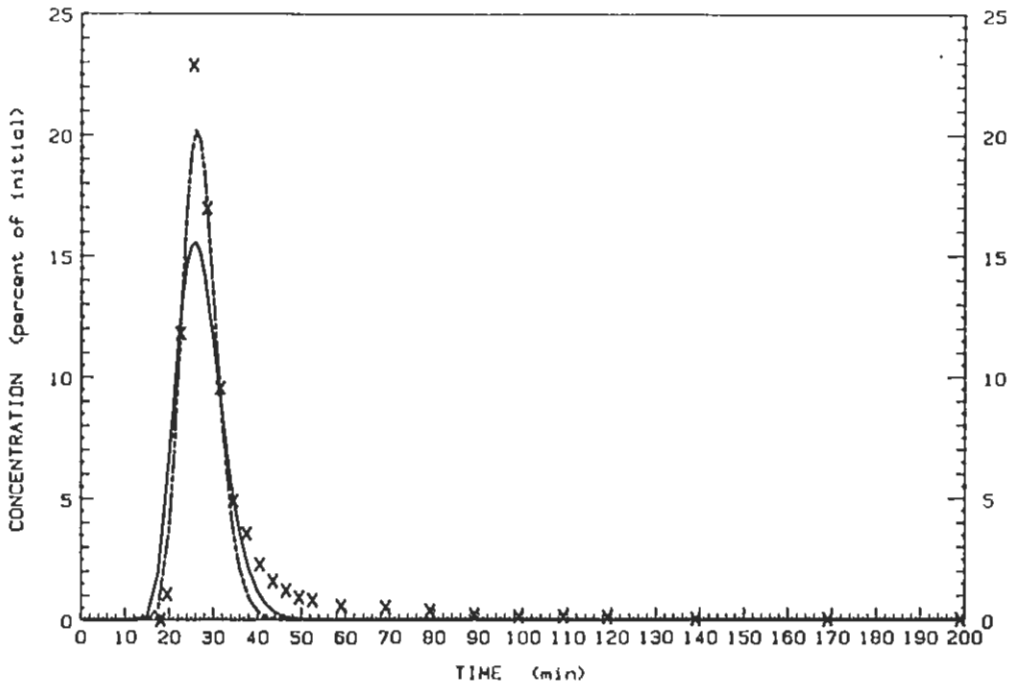

Figure 1c. Comparison of fit to data from experiment $2A_2$ (x) for the homogenous model (broken line) and the two zone model (solid line).

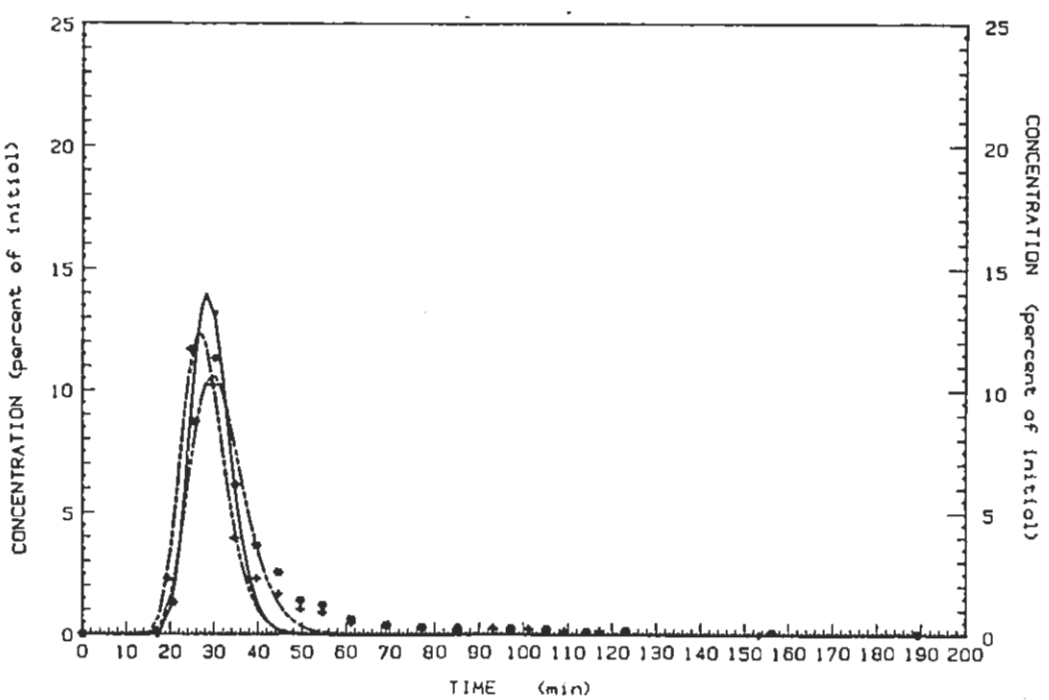

Figure 2. Scenario 2, breakthrough curve predicted from average fitted values of experiment 2A (solid line) for experiments $1A_1$ (+) and $1A_2$ (*). Curve fitted lines to the data itself are shown by the broken lines.

peak, the conclusion we first make is that the moisture content has increased within the column from the A to the B experiment even though the flow rate through the system is the same. By fitting the experimental data, v is found to be 2.86 cm/min which yields a moisture content of 13.7% (Table 3). Since D is approximately a linear function of v (Bear, (1976)) we recalculate D from the A experiment to be 4.86 cm^2. The broken line in Figure 3b shows the prediction for these values of D and v. It is clear that the prediction is too sharp and when D is fitted as well, we find it to have increased by about a factor two. The fitted curve is shown in Figure 3b (solid line) to be quite good.

Next we used the parameters of the A and B experiments to predict the B_{int} experiment where the water was intermittently applied (scenario 4). The average flow rate was lower by over a factor of 100. Thus we explore the common situation where parameters are obtained with high flow rates and then used in models under field conditions where the flow rates are much less.

The decrease in flow rate should cause a lowering of the moisture content and the dispersivity values. The procedure from the MOUSE program (Steenhuis et al., (1986)) is used to adjust the moisture content after which v is calculated from the known flux. The dispersion values were found again by taking the ratio of dispersivity and velocity to be a constant. These values for the steady state experiments were then used to predict the breakthrough for the intermittent experiment. Figure 4a shows that the predicted and observed values do not agree at all, again questioning the validity of the transportability of parameters between different experimental sets. Figure 4b shows how well the B_{int} data can be fitted by the solutions of both equation (1) and the two-zone model, once again demonstrating the ability of both models to fit experimental data well - once it is obtained!

We are faced with the same quandaries as for scenario 3 and 4 when trying to predict the results of the "C" experiments which, as it turns out, show completely different breakthrough curves than any of the "A", "B" or "B_{int}" experiments. So as to not belabor our point, we will not explore any additional validation scenarios.

DISCUSSION

Before we discuss our specific results it is useful to further consider the meaning of model validation for our case. Tsang, (1987) points out that any model is a simplification of reality and that it is a good representation of the real system if the model adequately yields results for specific observables of interest with the required accuracy and within the specific range of conditions. Thus, before we can judge how well the convection-dispersion model is validated we need

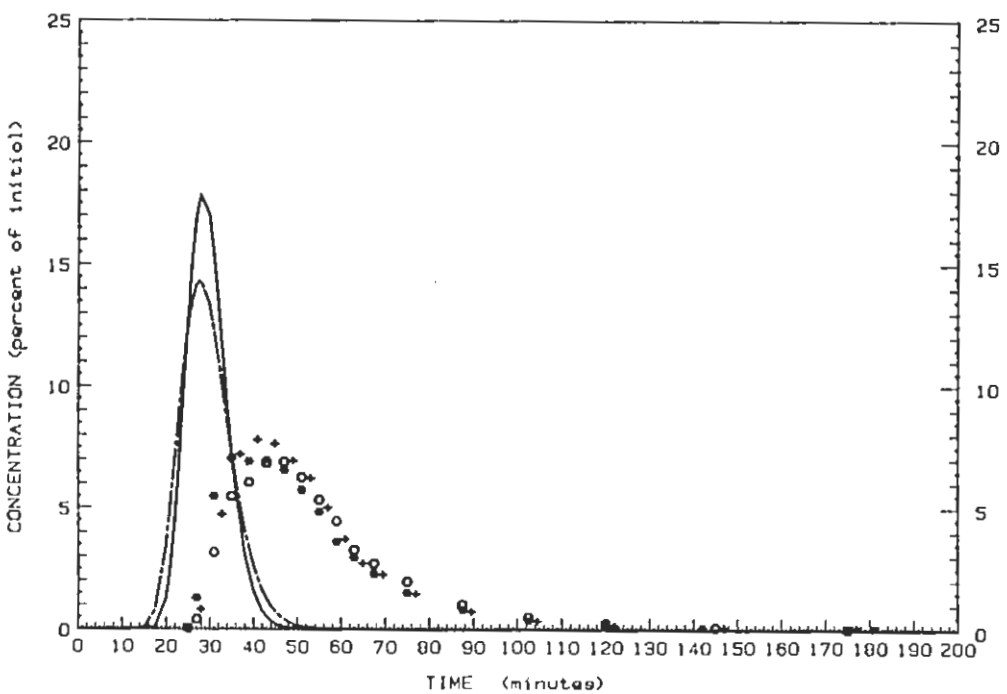

Figure 3a. Scenario 3, prediction of breakthrough curves for experiments $2B_1$ (+), $2B_2$ (*) and $2B_3$ (o) using average fitted parameters from 1A (broken line) and 2A (solid line).

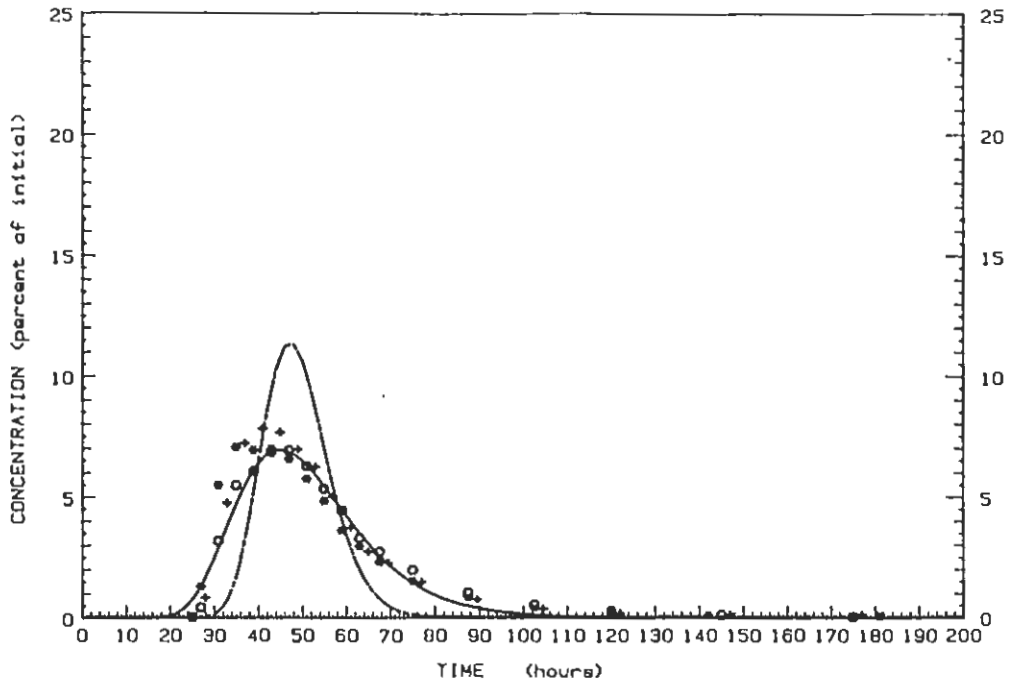

Figure 3b. Adjustment of prediction for apparent change in velocity (broken line) of breakthrough curves for experiments $2B_1$ (+), $2B_2$ (*), and $2B_3$ (o). Breakthrough data from experiment $2B_2$ is fitted to yield the solid line.

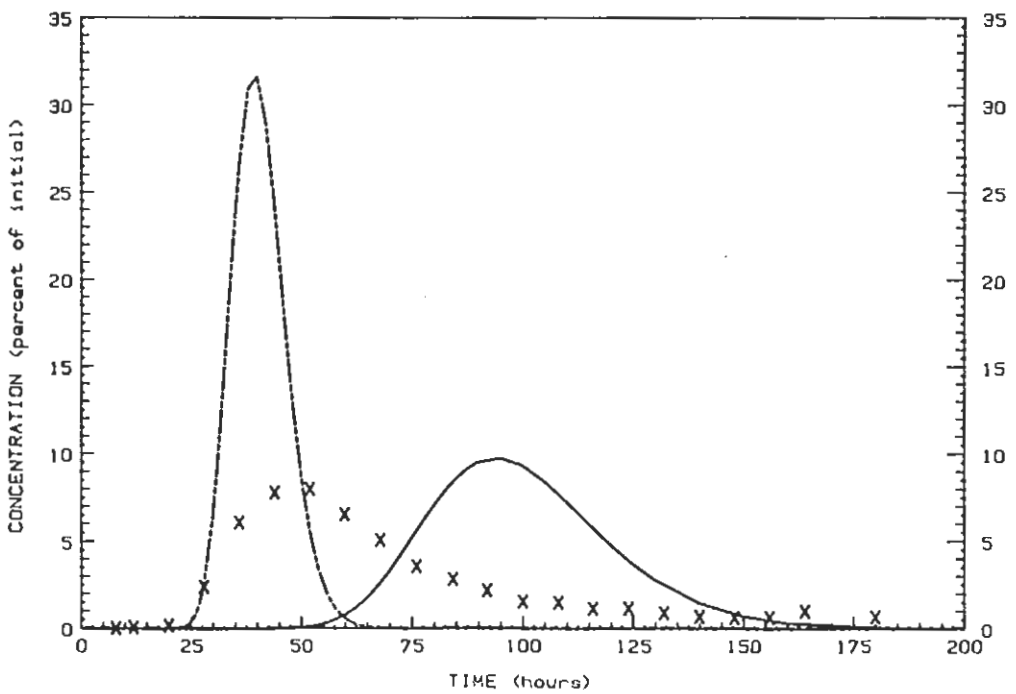

Figure 4a. Scenario 4, prediction of breakthrough curve for experiment $2B_{int}$ (x) using average fitted parameter values of experiment 2A (broken line) and 2B (solid line). Parameter values have been adjusted for the lower flow rate.

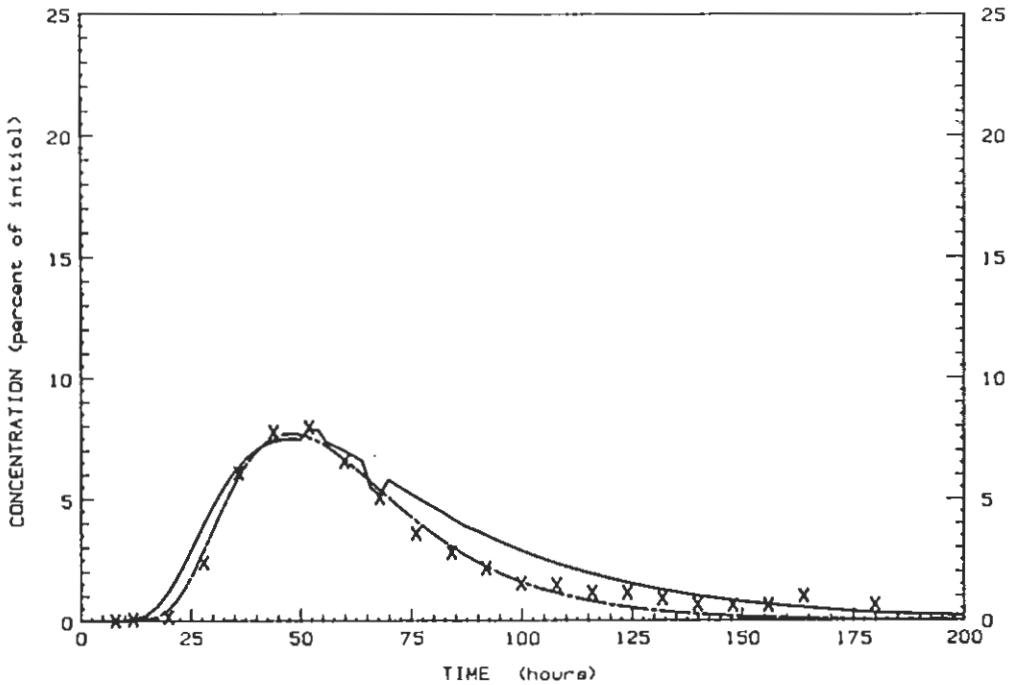

Figure 4b. Curve fit of $2B_{int}$ (x) data using the homogeneous model (brokon line) and two zone model (solid line).

to determine (Tsang, (1987)):

"(a) What are the observables of interest, (b) what is the accuracy required for prediction of these observables, and (c) what is the range of conditions for which the model is to be validated?"

For our experimental setup we can answer these questions as follows: (a) observables of interest are the concentration and fluxes of water at the ground water table (or the bottom of the column). (b) the required accuracy depends on the application for which it is used. In general, however we want to predict the time of arrival and concentration of the solute peak plus predict the "tails." Finally, (c) the range of conditions for which the model has to be valid should encompass the environmental situations that are encountered in the field where the model is applied. These include the experimental settings simulated in our laboratory experiments.

Tsang, (1987) differentiates between processes and model structure. He states that successful models need both proper model structure (e.g., the layered porous media) and the proper process identification (e.g., the convection-dispersion model with or without immobile water).

By using only scenarios 1 and 2 we would have concluded, considering the high regression coefficients, that our "process identification" described by the convection dispersion model applied to a "model structure" of an equivalent one-layer system was proper. We would probably have also assumed, based on traditional wisdom, that the model could be applied over a wide range of field conditions for which we have not explicitly validated the model.

When we consider scenario 3, in which we used the fitted parameters for the A experiment to predict the outflow concentrations in the B experiments, our conclusion must be revised: the processes identified may be proper for each experimental setting considered separately, however, the fitted parameters are not consistent between settings and the "process identification" and/or "model structure" are incorrect. Thus, the conditions for the B experiments fall outside the range of conditions for which the model is valid implying that a single one-layer convection-dispersion model does not model the physical processes occurring in our series of experiments, i.e., the model is nonphysical.

From an analysis of scenario 4 we also conclude that the model is nonphysical. Observations through the clear chamber walls of the path of the blue dye used as the solute in the experiments would also have proven this point. Glass et al., (1988) found that the two-layered system causes preferential flow of water through fingers in the coarse bottom layer due to wetting front instability. We would never have known this from

the breakthrough curves alone performed in one experimental setting. Under actual field conditions we most likely would have known only the concentration at the ground water. Thus, treatment of the vadose zone as a black box within which we apply the convection-dispersion model without the identification of all the basic processes can lead to serious errors. Other basic processes normally not considered include the temporal variation in surface connection of macropores due to the seasonal activity of earthworms or root growth.

Our results support and illustrate experimentally the validation philosophy developed by Rao et al., (1979) and Davidson et al., (1976); agreement between experimental data and computer output is a necessary but not sufficient condition for the validity of a model. Therefore, for curve fitting procedures to be a valid procedure in model verification a third step is necessary: the same set of parameters estimated from a given experimental setup should be used to predict experimental results obtained under many different conditions. Using their criteria, the one-layer model was not validated for the fine-over-coarse textured layered-soil system. The worrisome aspect is that extensive validation as carried out by us is unusual, and under most circumstances the procedures carried out under scenarios 1 and 2 would have been considered sufficient.

Currently there are few models available that are not based on some form of the convection-dispersion equation. At this time we have little choice but to use these models. Therefore, it is of utmost importance that the validation procedure be conducted as thoroughly as possible so that the range of model validity is shown precisely.

CONCLUSION

From this exercise we have learned that we cannot expect the convection-dispersion model to yield accurate predictions in all commonly occurring situations even if the model can be fitted quite well to most situations independently. Extensive model validation should be carried out and model prediction should be backed up by field monitoring under actual circumstances if the results are critical. The incorporation into the modeling effort of a cost benefit analysis that includes the cost of contaminant cleanup and litigation may give the justification needed for proper model validation. Lastly, a data set such as we have obtained emphasizes the fact that research on the fundamental processes actually occurring in the vadose zone is of critical importance.

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