# CHAPTER ELEVEN

## Field Parameterization of the Mobile/Immobile Domain Model

D.B. Jaynes and R. Horton

#### INTRODUCTION

It is clear from numerous field and laboratory experiments that solute movement is often poorly described by the classical advection-dispersion model. Rather, solute breakthrough curves frequently exhibit earlier arrival and more pronounced tailing than predicted by this model. These observations have spurred the development of conceptual models that specifically include physical nonequilibrium to more accurately depict solute movement. In the simplest version of these models, the waterfilled pore space is partitioned into two domains, a mobile domain, where water is free to move and solute movement is by advection and dispersion, and an immobile domain, where water is stagnant and solute moves only by diffusion.

Coats and Smith (1964) published an early version of this mobile/immobile domain (MIM) model which was later popularized by the work of van Genuchten and Wierenga (1976, 1977). For one-dimensional transport of a noninteracting, conservative solute, the MIM model can be written:

$$\theta_m \frac{\partial C_m}{\partial t} + \theta_{im} \frac{\partial C_{im}}{\partial t} = \theta_m D_m \frac{\partial^2 C_m}{\partial x^2} - q \frac{\partial C_m}{\partial x}$$
(11.1)

where  $\theta_m$  and  $\theta_{im}$  are the mobile and immobile volumetric water contents, the sum of which equals the total volumetric water content,  $\theta$ ;  $C_m$  and  $C_{im}$  are the solute concentrations in the mobile and immobile domains; t is time; x is distance;  $D_m$  is the hydrodynamic dispersion coefficient for the mobile domain; and q is Darcy flux. Exchange between the mobile and immobile domains is described by:

$$\theta_{im} \frac{\partial C_{im}}{\partial t} = \alpha (C_m - C_{im}) \tag{11.2}$$

where  $\alpha$  is a first-order mass transfer coefficient. Thus, the MIM model can account for more rapid solute transport because flow occurs in only a fraction of the waterfilled pore space and the model can account for the tailing observed in breakthrough curves via slow exchange of solute between the two domains (van Genuchten and Wierenga, 1977).

Equations 11.1 and 11.2 have been successfully applied to many laboratory column leaching studies. These studies have shown that both  $\theta_m$  and  $\alpha$  vary with the average pore water velocity, v (= q/ $\theta$ ), water content, and soil aggregate size (van Genuchten and Wierenga, 1977; Gaudet et al., 1977; Nkedi-Kizza et al., 1983; Kookana et al., 1993). Clothier et al. (1995) drew parallels between the apparent change in these transport parameters with the apparent change in the characteristic length determined from hydraulic conductivity measurements. Characteristic length typically decreases as the soil water pressure head decreases, presumably due to the emptying of the macro- and mesopores in the soil (Parlange, 1972; Jarvis and Messing, 1995).

Little information exists, however, as to the magnitude and behavior of MIM model parameters in field soils. In field tracer studies, the ratio  $\theta_m/\theta$  has been observed to vary from 1 (i.e., no preferential flow; Cassel, 1971) to 0.45–0.65 (Smettem, 1984; Gvirtzman and Magaritz, 1986), and even to as small as 0.25 in a weakly structured tropical soil (Seyfried and Rao, 1987) and a massive desert soil (Rice et al., 1986). Methods have been proposed for estimating  $\theta_{im}$  by equating it to the water remaining at some soil water pressure such as –33 kPa (Addiscott, 1977) or –202 kPa (Addiscott et al., 1986), or equating it to the residual water content from the water retention function (Jaynes et al., 1988b). However, these estimates appear to be soil-specific and have not been tested over an extensive range of soils.

Typically,  $\theta_m$  and  $\alpha$  are estimated from solute breakthrough curves where extended measurements of effluent concentration versus time are required. An inverse method such as described by Parker and van Genuchten (1984) is then used to estimate the model parameters giving the best fit (least sum-of-squares) to the data. Breakthrough curves are time-consuming to measure and are very difficult to conduct in the field. To fully characterize how  $\alpha$  and  $\theta_{im}$  vary by soil, management, and initial and boundary conditions, robust, easy-to-use measurement methods are required.

#### FIELD METHOD

As a first approach, we can use Equation 11.2 in conjunction with a simple tracer leaching study to get an estimate of  $\theta_m$  in field soils. If we infiltrate a solution containing a conservative, noninteracting tracer such as tritiated water into soil and sample the soil for tracer after a period of leaching, the average concentration in the soil, C, will be a combination of the tracer concentration in both the mobile and immobile domains. Assuming no immobile water and piston displacement of tracer within the mobile domain, the tracer concentration in the mobile domain,  $C_m$ , will equal the input concentration,  $C_o$ , and C will equal  $C_o$  behind the tracer front. If, however,  $\theta_{im} >$ 0, C will be less than the input concentration for soil initially tracer-free. By further assuming that  $\alpha$  is small compared to the leaching time for the tracer and that no tracer is initially present in the immobile water, from conservation of mass we find:

$$\theta_{im} = \theta \left( 1 - \frac{C}{C_o} \right) \tag{11.3}$$

This is the approach proposed by Clothier et al. (1992). They used a tension infiltrometer to apply a Br tracer to soil. This allowed them to vary the infiltration rate and resulting water content and quantify the effect on  $\theta_{im}$ . Using this method they found  $\theta_m/\theta$  to be 0.49 in a Manawatu fine sandy loam at an application pressure head

of -0.02 m. Further experiments by Clothier et al. (1995) showed that  $\theta_m/\theta$  was a function of the pressure head at which the tracer was applied, increasing from 0.41 at -0.02 m to 0.64 at -0.15 m of water head.

While a promising first approximation, assuming the  $\alpha = 0$  does not appear to be a realistic assumption in many cases. For example, Clothier et al. (1995) estimated  $\alpha$  to be 0.02 h<sup>-1</sup> over the first few days of tracer application. At this rate, measurable diffusion of solute into the immobile domain will occur in only a few hours. This estimate of  $\alpha$  is within the range of 0.001 to 10 h<sup>-1</sup> found from surveying a number of studies (Kookana et al., 1993). Thus, assuming  $\alpha \approx 0$  in most cases where tracer application exceeds about an hour will systematically over estimate  $\theta_m/\theta$  using Eq. 11.3.

Alternatively, we can assume  $\alpha$  is not negligible while still assuming piston displacement of tracer. A piston displacement assumption simplifies further analysis by removing the need to evaluate Eq. 11.1. Dispersion is ignored and for soil near the inlet boundary we assume that  $C_m = C_o$ . These assumptions allow for a focus on Eq. 11.2 which is solved to give:

$$\ln\left(1 - \frac{C}{C_o}\right) = \ln\left(\frac{\theta_{im}}{\theta}\right) - \frac{\alpha}{\theta_{im}}t^*$$
(11.4)

where  $t^* = t - \ell/v$  and is defined as the time required for the tracer front to reach the depth of sampling,  $\ell$ . Substituting for  $t^*$  in Eq. 11.4 gives:

$$\ln\left(1 - \frac{C}{C_o}\right) = \ln\left(\frac{\theta_{im}}{\theta}\right) + \frac{l\alpha\theta_m}{\theta_{im}q} - \frac{\alpha}{\theta_{im}}t$$
(11.5)

Thus by regressing  $\ln(1-C/Co)$  versus time, both  $\alpha$  and  $\theta_{im}$  can be found from the resulting intercept and slope.

This is the approach first proposed by Jaynes et al. (1995), where they infiltrated a sequence of conservative, noninteracting tracers over time and measured the resident concentrations in a shallow soil sample. By again using a tension infiltrometer to apply the tracers, the dependence of  $\alpha$  and  $\theta_{im}$  on the infiltrometer tension (and thus v and  $\theta$ ) can be determined.

In their approach, Jaynes et al. (1995) used four different tracers rather than repeated measurements with a single tracer. An advantage to using multiple tracers is that only one soil sample need be taken, eliminating sample-to-sample variability. A disadvantage of the technique is that the transport properties of the different tracers may not be identical. Jaynes et al. (1995) used Br- and the fluoridated benzoates, pentafluorobenzoate, *o*-trifluoromethylbenzoate, and 2,6-difluorobenzoate, which are known to have near identical transport properties in many soils (Jaynes, 1994) and similar aqueous diffusion coefficients (Bowman and Gibbens, 1992; Benson and Bowman, 1994).

Jaynes et al. (1995) found good linearity for the data (Figure 11.1) when resident tracer concentration was plotted vs. time as given in Eq. 11.5. Discrepancy between the measured and predicted behavior may have been due to experimental limitations such as difficulty in measuring the small differences in tracer concentration or non-identical transport behavior of the individual tracers. This latter possibility can be compensated for by alternating the order of tracer application during replicate determinations. Values determined for  $\alpha$  and  $\theta_{im}$  by Jaynes et al. (1995) were well within the range observed by others in laboratory column experiments.

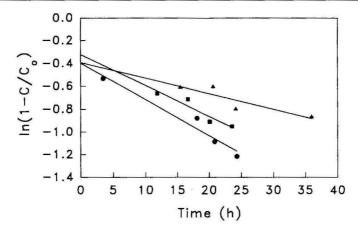


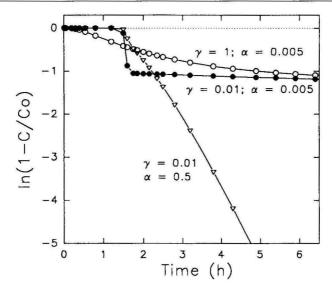
Figure 11.1. Examples of resident solute concentrations from three replicate leaching experiments plotted as per Eq. 11.5 and the best fit lines to the data. From Jaynes, D.B., *Soil Sci. Soc. Am. J.*, 59:352–356, 1995. With permission.

The sequential tracer technique can potentially be used for measuring the distribution of  $\alpha$  and  $\theta_{im}$  in field soils. While not as simple to use as the single tracer method of Clothier et al. (1992), it retains many of the advantages (a single soil sample is taken and total experimental time is relatively short), while giving estimates of the additional parameter,  $\alpha$ . In its simplest form, only two tracers need be applied, although the use of multiple tracers allows for the confirmation of log-linear behavior predicted by Eq. 11.5. If accurate, the method will make possible the determination on how  $\alpha$ and  $\theta_{im}$  vary as functions of soil type, crop, and tillage over a range of wetting heads.

#### EVALUATION OF MULTIPLE TRACER APPROACH

While Jaynes et al. (1995) showed that Eq. 11.5 gave reasonable estimates of  $\alpha$  and  $\theta_{im}$ , they did not compare these estimates to independent estimates determined by other means such as curve fitting of breakthrough curves (inverse method). Nor did they evaluate the range over which the assumptions leading to Eq. 11.5 are valid. A direct approach would be to compare Eq. 11.5 to the analytical solution of Eqs. 11.1 and 11.2 such as given by Parker and van Genuchten (1984). However, we have been unable to reformulate their solution into a form directly comparable to Eq. 11.5. As an alternative, we can compare the estimates of  $\alpha$  and  $\theta_{im}$  given by Eq. 11.5 when applied to data generated from the complete analytical solution with known input values.

Figure 11.2 shows the results of three simulations using the analytical solution to Eqs. 11.1 and 11.2 (Parker and van Genuchten, 1984). In these simulations, v was set to 1 cm hr<sup>-1</sup>,  $\theta_m/\theta$  to 0.66 and the resident concentration vs. time at a depth of 2 cm below the surface was calculated. Three combinations of dispersivity,  $\gamma$  (= D/v), and  $\alpha$  were used. In the first simulation,  $\gamma = 0.01$  cm and  $\alpha = 0.005$  h<sup>-1</sup>. After about 1.7 h, ln(1–C/C<sub>o</sub>) vs. time is well represented by a straight line as described by Eq. 11.5 (Figure 11.2). In the second simulation,  $\alpha$  was again set to 0.005 h<sup>-1</sup> and  $\gamma$  was increased to 1 cm. Plotting the results of the simulations in Figure 11.2 results in a concave-upward curve that is poorly represented by a straight line. At this higher dispersivity, the assumption of piston displacement of solute is not valid and transport is poorly described by Eq. 11.5. Finally, Figure 11.2 shows the results of a simulation where  $\gamma = 0.01$  cm and  $\alpha = 0.5$  h<sup>-1</sup>. Again, the resulting curve is poorly described by Eq. 11.5, being



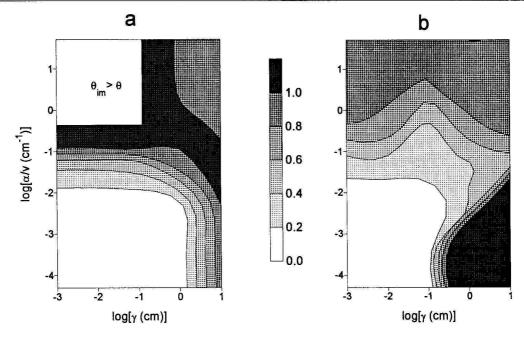
**Figure 11.2.** Examples of simulated resident concentration data for a depth of 2 cm generated from the analytical solution to the MIM model for a  $\theta_m/\theta$  ratio of 0.66 and a water flux of 0.5 cm h<sup>-1</sup> and plotted as per Eq. 11.5. Values on figure are for dispersivity,  $\gamma$ , in cm and the inter-domain solute transfer coefficient,  $\alpha$ , in h<sup>-1</sup> used in each simulation.

concave downward. Thus even at a low dispersivity, the rapid exchange between the mobile and immobile domains caused by setting  $\alpha$  high negates the assumption that  $C_m = C_o$  made in developing Eq. 11.5.

Using the analytical solution to compute soil solution concentration data for a range of parameter values and applying Eq. 11.5 to the generated data, we can determine the range in conditions for which calculated values of  $\alpha$  and  $\theta_{im}$  are accurate. We compute a relative error for the calculated parameters by dividing the absolute difference between the known parameter value used in the simulation and the value calculated from Eq. 11.5, by the known value. Figure 11.3a shows the relative error in calculated values of  $\theta_{im}$  over a range of  $\log(\gamma)$  and  $\log(\alpha/v)$  values and a  $\theta_{im}/\theta$  ratio of 0.33. Relative errors in the computed value of  $\theta_{im}$  are less than 0.2 over a wide range of  $\gamma$  and  $\alpha/v$  values. However, as  $\gamma$  increases above 1 cm the relative error increases rapidly for all values of  $\alpha/v$ . Likewise, as  $\alpha/v$  increases beyond 0.01 cm<sup>-1</sup>, the relative error increases rapidly. For low values of  $\theta_{im}$  that are greater than the value of  $\theta$ .

Figure 11.3b is the graph of the relative error in  $\alpha$  calculated from Eq. 11.5. Low relative errors are found for values of  $\gamma$  less than 0.1 cm and for  $\alpha/\nu$  values less than 0.03 cm<sup>-1</sup>. Unlike the results for  $\theta_{im}$ , reasonable values of  $\alpha$  are still calculated for low  $\gamma$  values and  $\alpha/\nu$  ratios greater than 0.03 cm<sup>-1</sup>, the values never being worse than about a factor of 2 in error. Decreasing the  $\theta_m/\theta$  ratio used in the simulations, enlarges the regions in Figure 11.3 giving reasonable parameter values; increasing the ratio reduces these regions.

Based on comparisons with the complete solution to the MIM model, Eq. 11.5 would appear to give reasonable estimates of  $\alpha$  and  $\theta_{im}$  over a restrictive range of conditions. However, a survey of the literature shows that most reported values of  $\alpha/v$  are  $\leq 0.1 \text{ cm}^{-1}$  (Kookana et al., 1993), which corresponds to the lower half of Figure 11.3. Thus, it would appear that expected  $\alpha/v$  ratios will not appreciably limit the applicability of Eq. 11.5.



**Figure 11.3.** Map of the relative error in the estimated value of (a)  $\theta_{im}$  and (b)  $\alpha$  as functions of  $\log(\gamma)$  and  $\log(\alpha/\nu)$ . Data were generated from the analytical solution of the MIM model and known model parameters with a  $\theta_m/\theta$  ratio of 0.66 and a simulation depth of 2 cm. Parameter estimates were obtained from applying Eq. 11.5 to the generated data. Blanked space in upper left corner of (a) represents values where computed  $\theta_{im}$  values exceed  $\theta$ .

Representative values for  $\gamma$  are less certain. In laboratory column studies, reported values for  $\gamma$  have ranged from 0.16 to 2.0 cm (van Genuchten and Wierenga, 1977; Gamerdinger et al., 1990; Kookana et al., 1993). Over this range of  $\gamma$  values, Eq. 11.5 should give reasonable estimates of  $\alpha$  and  $\theta_{im}$  (Figure 11.3). However, estimates of  $\gamma$  based on field-scale experiments are usually 10 to 100 times larger (Jaynes et al., 1988a; Yasuda et al., 1994), well outside the range of applicability for Eq. 11.5. These large  $\gamma$  values may in part be due to the greater heterogeneity of soil over the larger spatial scales used, and will limit the accuracy of Eq. 11.5. However, the sequential tracer approach may still be helpful since no other practical method exists for estimating the MIM transport parameters in the field.

#### LABORATORY EVALUATIONS

The applicability of Eq. 11.5 can be evaluated from leaching studies using laboratory soil columns by comparing estimates based on Eq. 11.5 vs. estimates obtained by applying inverse methods. By applying a sequence of tracers to a soil column over time,  $\alpha$  and  $\theta_{im}$  can be calculated using Eq. 11.5 and resident solute concentrations from within the soil column. Similarly, independent estimates for  $\alpha$  and  $\theta_{im}$  can be made by applying inverse methods to the solute concentrations in the column outflow vs. time (Parker and van Genuchten, 1984). Inverse methods applied to solute breakthrough curves are typically used to estimate the parameter values in Eqs. 11.1 and 11.2 (van Genuchten and Wierenga, 1977; Seyfried and Rao, 1987).

Column #	Soil Material	ρ	θ	v
		Mg m <sup>-3</sup>	kg kg⁻¹	cm h-1
1	Florida beach sand <sup>a</sup>	1.54	0.40	32.8
2	Clarion Ap, sicl <sup>b</sup>	0.94	0.56	41.4
3	Clarion C, sicl <sup>b</sup>	0.94	0.49	16.2
4	Tama Ap, I <sup>b</sup>	0.96	0.59	45.0
5	Tama C1g, 🖻	0.96	0.49	35.3

Table 11.1. Soil, Bulk Density ( $\rho$ ), Water Content ( $\theta$ ), and Pore-Water Velocity (v) for Each Column.

<sup>a</sup> 0.5–1 mm sieve fraction.

b 1–2 mm sieve fraction.

Five 12.5-cm long columns were packed with different soil materials (Table 11.1). Details of these and other column experiments can be found in Lee et al. (1998). In each experiment, the soil was first saturated with a 0.4 mM CaCl<sub>2</sub> solution. The columns were then leached with the same solution under a slight ponded head until steady flow conditions were achieved. A sequence of solutions were then introduced at the top of each column. The first solution contained 0.3 mM CaCl<sub>2</sub> and 0.1 mM of either pentafluorobenzoate (PFBA), *o*-trifluoromethylbenzoate (TFMBA), 2,6-difluorobenzoate (DFBA), or 2,3,6-trifluorobenzoate (TFBA) tracer. After leaching the column with about 1 pore volume of the first solution, a second solution was applied containing 0.2 mM of CaCl<sub>2</sub>, 0.1 mM of the first benzoate tracer, and 0.1 mM of a second benzoate tracer. The process was repeated until the final solution contained no CaCl<sub>2</sub> and the four benzoate tracers at a concentration of 0.1 mM each. Outflow containing the tracers was collected from the columns with a fraction collector. Following infiltration of the last tracer, the columns were sectioned in 1 cm increments and the tracers extracted and measured to calculate the resident tracer concentration vs. depth.

Figure 11.4 shows the concentrations of the four tracers in outflow from column 4 vs. time, normalized by the input concentrations. Breakthrough curves for the other columns were similar. Each breakthrough curve had early arrival of tracer indicative of physical nonequilibrium processes. The breakthrough curve for each tracer was normalized by the input concentration and adjusted so that t=0 when the individual tracer was first applied to the column. The four breakthrough curves were then combined and the best fit values for the parameters D,  $\alpha$ , and  $\theta_{im}$  in Eqs. 11.1 and 11.2 found by inverse methods using the program CXTFIT (Parker and van Genuchten, 1984).

Resident concentrations for the four tracers in column 4 are shown in Figure 11.5. Tracer profiles in the other columns were similar. Relative concentrations were all less than 1, indicating the presence of immobile water in each column. At most depths, relative concentrations were greater for tracers applied the longest, indicative of transfer processes occurring between the mobile and immobile domains. Finally, the last tracer applied showed considerable dropoff in concentration with depth and clearly shows a zone where dispersion processes are important.

Equation 11.5 was applied to the resident concentration data. Because insufficient leaching of the last applied tracer would cause interference from dispersion processes, only the concentrations from the top layers were used. We also discarded data from the top 1-cm layer in each column since this layer had bulk densities considerably lower than the rest of the column. Figure 11.6 shows the resident concentrations in the four layers of column 4 plotted as  $ln(1-C/C_o)$  vs. time and the resulting best fit line to each layer. For each soil layer straight lines fit the data reasonably well.

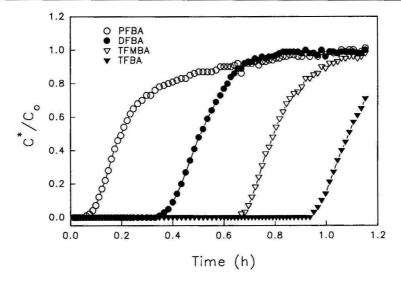


Figure 11.4. Effluent concentrations, C<sup>\*</sup>, normalized by input concentrations, C<sub>o</sub>, vs. time of 4 sequentially applied benzoate tracers in column 4.

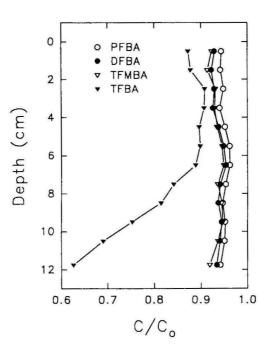
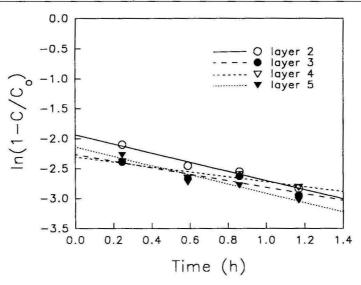


Figure 11.5. Average pore-water concentrations vs. depth normalized by the input concentrations of 4 benzoate tracers sequentially applied to column 4.

We can compare values of  $\alpha$  and  $\theta_{im}$  calculated using an inverse method (CXTFIT) and the outflow data to values calculated using Eq. 11.5 and the resident solute concentration data (Figure 11.7). For the inverse method, the best fit value and its computed 95% confidence limit is plotted. For the regression method, the four estimates from the top four layers are plotted. Calculating  $\gamma$  from the D values estimated by the



**Figure 11.6.** Resident concentrations of tracers within layers 2–5 of column 4 plotted as per Eq. 11.5 and the best fitting lines to the data.

inverse method, we find that the experimental conditions for all columns except 1 were marginal for using Eq. 11.5 to estimate  $\alpha$  and  $\theta_{im}$  (Figure 11.3). Even so, the two estimation methods gave similar estimates of  $\alpha$  and  $\theta_{im}/\theta$  for each column except column 5 where the inverse estimate of  $\theta_{im}/\theta$  is greater than that found using Eq. 11.5.

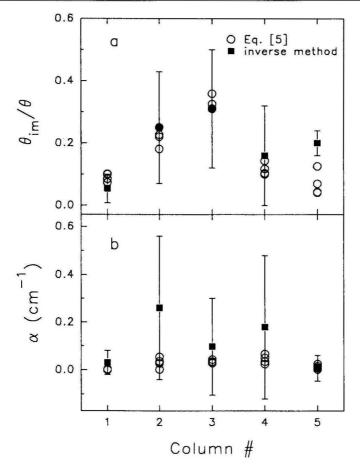
#### FIELD APPLICATIONS

Eq. 11.5 was applied to two different field sites in central Iowa. Tension infiltrometers were used in both experiments to introduce a sequence of tracer solutions at the soil surface. The first experiment used only a single pressure head, -0.03 m. The second experiment included infiltration at four pressure heads, 0.01, -0.03, -0.06, and -0.15 m. The first experiment included a transect of 47 infiltration sites. The second experiment was set as a grid of 40 infiltration sites with 10 at each tension randomly assigned. Full details of the experiments can be found in Casey (1996), Casey et al. (1997), and Casey et al. (1998).

Figure 11.8a presents the spatial distribution of the  $\theta_{im}/\theta$  values obtained from the first field experiment. The median of  $\theta_{im}/\theta$  was 0.627, the mean 0.646, and standard deviation 0.065. Based upon semivariogram analysis, no spatial correlation of  $(\theta_{im}/\theta)$  was detected (i.e., a pure nugget semivariogram). The values of  $\theta_{im}/\theta$  determined in this experiment fall within the range of values reported by other investigators (van Genuchten et al., 1977; Nkedi-Kizza et al., 1983, 1984; Smettem, 1984; Gvirtzman and Magaritz, 1986; Rice et al., 1986). However, the average of these field values is on the high side of earlier reported values.

Figure 11.8b shows the spatial distribution of the  $\alpha$  values obtained from the first field experiment. The median  $\alpha$  was 0.078 h<sup>-1</sup>, the mean 0.09 h<sup>-1</sup>, and the standard deviation 0.054 h<sup>-1</sup>. Semivariogram analysis indicated no spatial correlation. The values of  $\alpha$  obtained in this experiment were similar to those reported from earlier laboratory studies (Kookana et al., 1993).

Figure 11.9 shows a relationship between  $\alpha$  and pore water velocity. The graph contains data from earlier laboratory studies as well as the Casey et al. (1997) field

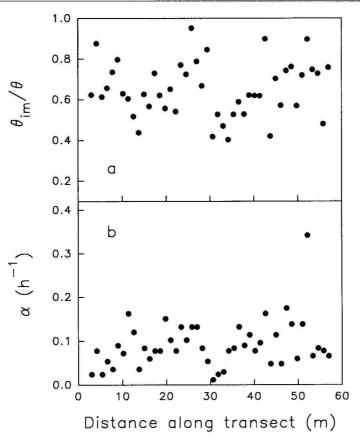


**Figure 11.7.** Comparison of solute transport parameters (a)  $\theta_{im}/\theta$  and (b)  $\alpha$  estimated from both solute breakthrough curves and inverse methods, and the resident concentrations in layers 2–5 and Eq. 11.5, for 5 column experiments. Error bars on values from inverse method represent the 95% confidence limits of the estimates.

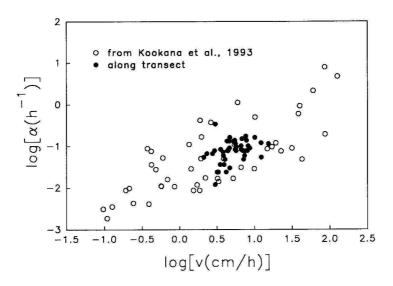
data. The laboratory and field data indicate a similar relationship between  $\alpha$  and pore water velocity. The field estimates of  $\alpha$  based upon Eq. 11.5 are of similar range and of similar relationship to pore-water velocity as reported by others from lab studies. This finding supports the usefulness of the sequential tracer method for determining field transport parameters.

Figure 11.10a shows values of  $\theta_{im}/\theta$  as a function of pressure head from the second field experiment. Mean and standard deviation of  $\theta_{im}/\theta$  for pressure heads of 0.01, -0.03, -0.06, and -0.15 m were 0.40 (0.17), 0.27 (0.11), 0.22 (0.04), and 0.35 (0.20), respectively. Angulo-Jaramillo et al. (1996) also reported fluctuations in  $\theta_{im}/\theta$  values with pressure head.  $\theta_{im}$  was largest at a pressure head of 0.01 m and was nearly constant for the other three pressure heads. The measured total water contents for pressure heads of 0.01, -0.03, -0.06, and -0.15 m were 0.41, 0.35, 0.34, and 0.34, respectively. Thus, total water content and immobile water content had similar trends with pressure head.

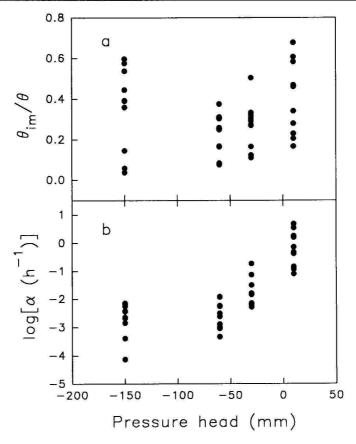
Figure 11.10b shows values of  $\alpha$  as a function of pressure head for the second field experiment. Mean and standard deviation of  $\alpha$  for pressure heads of 0.01, -0.03, -0.06, -0.15 m were 1.3 (1.5), 0.036 (0.054), 0.0044 (0.0041), and 0.0033 (0.0024) h<sup>-1</sup>, respec-



**Figure 11.8.** Values of (a)  $\theta_{im}/\theta$  and (b)  $\alpha$  measured along a field transect. From Casey, F.X.M. et al., *Soil Sci. Soc. Am. J.*, 61:1030–1036, 1997. With permission.



**Figure 11.9.**  $\alpha$  versus v values measured along a transect compared to values summarized from earlier column experiments by Kookana et al., 1993. From Casey, F.X.M. et al., *Soil Sci. Soc. Am. J.*, 61:1030–1036, 1997. With permission.



**Figure 11.10.** Values of (a)  $\theta_{im}/\theta$  and (b)  $\alpha$  versus infiltrometer pressure head measured at 40 locations in a field (Casey, 1996).

tively. As found by others (Kookana et al., 1993), the  $\alpha$  values were correlated with infiltration flux and thus pore water velocity and pressure head. The average ratios for  $\alpha/v$  for these same pressure heads were 0.015, 0.012, 0.003, and 0.006 cm<sup>-1</sup>. Thus for dispersivities less than about 1 cm, the calculated values for  $\alpha$  and  $\theta_{im}$  should be no worse than 20% in error (Figure 11.3).

We can compare the values of  $\alpha$  and  $\theta_{im}/\theta$  found at a pressure head of -0.03 m in the two field experiments directly. At a probability of 0.05, the  $\alpha$  values in the two field studies were not significantly different. However, the  $\theta_{im}/\theta$  values were significantly different at a probability of 0.05. The two field sites differed in a couple of important ways. Tillage differed, no-till versus ridge-till. Corn growth stage also differed at the time of measurements. Both soils were glacial till, but soil types differed. Similar  $\alpha$  values implies similar microporosity makeup of the two field soils. Differing  $\theta_{im}/\theta$  values implies differences in the macroporosity of the field soils. Transport parameter comparisons between the two sites imply that  $\alpha$  is somewhat independent of soil management practices while  $\theta_{im}/\theta$  responds to soil management practices.

#### SUMMARY

A simple method for estimating immobile water content and mass exchange coefficient for the MIM model has been presented and evaluated. The method is useful for laboratory and field applications. A numerical study indicates the experimental conditions to which the method can be best applied. Laboratory tests indicate that the simple method provides values of  $\alpha$  and  $\theta_{im}$  similar to those obtained from solute breakthrough curve analysis. This method is the only practical method available for determining these solute transport parameters in the field. Finally, because tension infiltrometers are used, field soil hydraulic properties, water retention and unsaturated hydraulic conductivity, also can be determined at the same time that the mass exchange coefficient and immobile water content are determined.

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### CONTRIBUTORS

T.M. Addiscott Rothamsted Experimental Station Harpenden, Herts AL5 2JQ United Kingdom

A.C. Armstrong ADAS Land Research Centre Gleadthorpe, Meden Vale Mansfield, Notts NG20 9PF United Kingdom

H.W.G. Booltink Wageningen Agricultural University Department of Soil Science and Geology 6700 AA Wageningen The Netherlands

J. Bouma Wageningen Agricultural University Department of Soil Science and Geology 6700 AA Wageningen The Netherlands

Mark L. Brusseau Department of Soil, Water and Environmental Science and Department of Hydrology and Water Resources University of Arizona Tucson, AZ 85721

W. Chen Novartis Environmental Safety Department P.O. Box 18300 Greensboro, NC 27419-8300

Brent E. Clothier Environment Hort Research PB 11-030 Palmerston North New Zealand J.H. Dane Department of Agronomy and Soils Auburn University Auburn, AL 36849-5412

Liliana Di Pietro Unité de Science du Sol INRA Domaine St. Paul Site Agroparc 84914 Avignon, Cedex 9 France

P. Droogers
Wageningen Agricultural University
Department of Soil Science and Geology
6700 AA Wageningen
The Netherlands

Robert B. Edis Department of Agriculture and Resource Management The University of Melbourne Parkville, Victoria 3052 Australia

Markus Flury Department of Crop and Soil Sciences Washington State University Pullman, WA 99164

Simon N. Gleyzer Department of Environmental Sciences and Engineering University of North Carolina at Chapel Hill Chapel Hill, NC 27599

Steve R. Green Environment Group HortResearch, PB 11-030 Palmerston North New Zealand Jin-Ping Gwo Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831

Lee K. Heng Department of Agriculture and Resource Management The University of Melbourne Parkville, Victoria 3052 Australia

Robert Horton Department of Agronomy Iowa State University Ames, IA 50011

Tissa H. Illangasekare Department of Civil Engineering University of Colorado Boulder, CO 80309-0428

Paul T. Imhoff Department of Civil and Environmental Engineering University of Delaware Newark, DE 19716

Philip M. Jardine Earth and Atmospheric Sciences Section Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831-6038

Nicholas Jarvis Department of Soil Science Swedish University of Agricultural Science Box 7014 S-750 07 Uppsala Sweden

Dan B. Jaynes USDA-ARS National Soil Tilth Laboratory 2150 Pammel Drive Ames, IA 50011 William A. Jury Department of Soil and Environmental Sciences University of California Riverside, CA 92521

Eileen J. Kladivko Agronomy Department Purdue University West Lafayette, IN 47907

P.B. Leeds-Harrison Cranfield University School of Agriculture Food and Environment Silsoe, Beds MK45 4DT United Kingdom

Feike J. Leij USDA-ARS U.S. Salinity Laboratory 450 West Big Springs Road Riverside, CA 92507-4617

H.H. Liu Environmental Systems Engineering Department Clemson University Clemson, SC 29634

R.J. Luxmoore Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831-6038

Liwang Ma Agronomy Department Louisiana State University Baton Rouge, LA 70803

Robert S. Mansell P.O. Box 110290 Department of Soil and Water Science University of Florida Gainesville, FL 32611-0290

Cass T. Miller Department of Environmental Sciences and Engineering University of North Carolina Chapel Hill, NC 27599 Rachel O'Brien Department of Geology Washington State University Pullman, WA 99164-2812

Andrew S. Rogowski Department of Agronomy 445 A.S.I. Building The Pennsylvania State University University Park, PA 16802-3504

Dave R. Scotter Soil Science Department Massey University Palmerston North New Zealand

H.M. Selim Agronomy Department Sturgis Hall Louisiana State University Baton Rouge, LA 70803

Dilip Shinde Soil and Water Science Department University of Florida Gainesville, FL 32611 Nobuo Toride Department of Agricultural Sciences Saga University Saga 840 Japan

Iris Vogeler Environment Group HortResearch, PB 11-030 Palmerston North New Zealand

R.J. Wagenet Department of Agronomy Cornell University Ithaca, NY 14853

Robert E. White Department of Agriculture and Resource Management The University of Melbourne Parkville, Victoria 3052 Australia

Glenn V. Wilson Desert Research Institute 755 E. Flamingo Rd. Las Vegas, NV 89119-0040