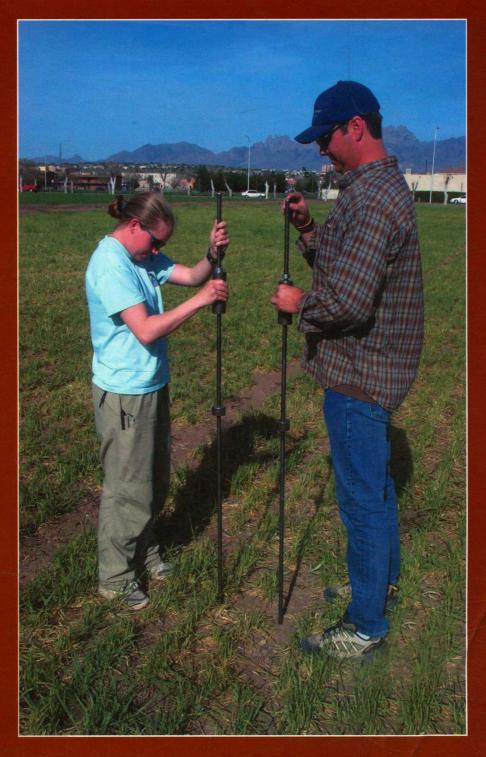
SSSAJ

Soil Science Society of America Journal



Soil Science Society of America Journal

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Keep authors anonymous from reviewers by listing title, author(s), author-paper documentation, and acknowledgments on a detachable title page. Repeat manuscript title on the abstract page.

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 A short title not exceeding 12 words. The title should accurately identify and describe the manuscript content.

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Abstract. An informative, self-explanatory abstract, not exceeding 250 words (150 words for notes), must be supplied on a separate page. It should specifically tell why and how the study was made, what the results were, and why they were important. Use quantitative terms. The title should be repeated on top of the abstract page without author identification.

Tables. Each table must be on a separate page and numbered consecutively. Do not duplicate matter that is presented in charts or graphs. Use the following symbols for footnotes in the order shown: † † 8 ¶ # †† †† etc

†, ‡, §, ¶, #, ††, ‡‡, . . . etc.

The symbols *, **, and *** are always used to show statistical significance at 0.05, 0.01, and 0.001 levels, respectively, and are not used for other footnotes. Spell out abbreviations on first mention in tables, even if the abbreviation is defined in the text (i.e., a reader should be able to understand the table contents without referring back to the text).

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- 2. Arrange the list alphabetically by the names of the first authors and then by the second and third authors.
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munications or privileged data, should be cited in the text in parenthetical form.

8. Chapter references from books must include, in order, authors, year, chapter or article title, page range, editor(s), book title, publisher, and city.

9. Symposium proceedings should include editor, date and place of symposium, publisher, and page numbers.

Style Guidelines

All soils discussed in publications should be identified according to the U.S. soil taxonomic system the first time each soil is mentioned. The Latin binomial or trinomial and authority must be shown for all plants, insects, pathogens, and animals when first mentioned. Both the accepted common name and the chemical name of pesticides must be provided. SI units must be used in all manuscripts. Corresponding metric or English units may be added in parentheses at the discretion of the author. If a commercially available product is mentioned, the name and location of the manufacturer should be included in parentheses after first mention.

Official Sources.

 Spelling: Webster's New Collegiate Dictionary
 Amendments to the U.S. system of soil taxonomy (Soil Survey) Staff, 1975) have been issued in the National Soil Survey Handbook (NRCS, 1982-1996) and in Keys to Soil Taxonomy (Soil Survey Staff, 1996). Updated versions of these and other resources are available at http://www.statlab.iastate.edu/soils/index.

3. Scientific names of plants: A Checklist of Names for 3000 Vascular Plants of Economic Importance (USDA Agric. Handb. 505, see also the USDA Germplasm Resources Information Network database, http://www.ars-grin.gov/npgs/searchgrin.html)

4. Chemical names of pesticides: Farm Chemicals Handbook

(Meister Publishing, revised yearly) Soil series names: Soil Series of the United States, Including Puerto Rico and the U.S. Virgin Islands (USDA-SCS Misc. Publ. 1483, http://www.statlab.iastate.edu:80/soils/osd)

6. Fungal nomenclature: Fungi on Plants and Plant Products in

the United States (APS Press)

Journal abbreviations: Chemical Abstracts Service Source Index (American Chemical Society, revised yearly)

8. The Glossary of Soil Science Terms is available both in hard copy (SSSA, 1997) and on the SSSA Web page (www.soils.org/ sssagloss/). It contains definitions of more than 1800 terms, a procedural guide for tillage terminology, an outline of the U.S. soil classification system, and the designations for soil horizons and layers.

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Authors have three months to make revisions and return their manuscripts following reviewer and associate editor comments. If not returned within three months, the manuscript will be released; it must then be resubmitted as a new paper.

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In general, four manuscript pages will equal one printed page. For space economy, Materials and Methods, long Literature Reviews, theory, soil or site descriptions, etc., footnotes, tables, figure captions, and references are set in small type. Each table and figure will usually take 1/4 of a printed page. For tabular matter, 9 lines of typewritten matter equal 1 column-inch of type. Allow also for rules and spacing. Tables with more than 35 units (including space between words) in a horizontal line can rarely be set 1 page-column wide. The depth of a printed figure will be in the same proportion to the width (1 column = 8.5 cm; 2 column = 17.2 cm) as that of the corresponding dimensions in the original drawing.

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Questions?

Send your questions to Nicholas Rhodehamel, Managing Editor, SSSAJ (nrhodehamel@agronomy.org).

February 1, 2002

Conversion Factors for SI and non-SI Units

To convert Column 1 into Column 2, multiply by	Column 1 SI Unit	Column 2 non-SI Unit	To convert Column into Column 1, multiply by
		ength	manips, oy
0.621	kilometer, km (10 ³ m)	mile, mi	1.609
1.094	meter, m	yard, yd	0.914
3.28	meter, m	foot, ft	0.304
1.0	micrometer, μm (10 ⁻⁶ m)	micron, μ	1.0
3.94×10^{-2}	millimeter, mm (10^{-3} m)	inch, in	25.4
10	nanometer, nm (10 ⁻⁹ m)	Angstrom, Å	0.1
	A	Area	
2.47	hectare, ha	acre	0.405
247	square kilometer, km ² (10 ³ m) ²	acre	4.05×10^{-3}
0.386	square kilometer, km ² (10 ³ m) ²	square mile, mi ²	2.590
2.47×10^{-4}	square meter, m ²	acre	4.05×10^{3}
10.76	square meter, m ²	square foot, ft ²	9.29×10^{-2}
1.55×10^{-3}	square millimeter, mm ² (10 ⁻³ m) ²	square inch, in ²	645
	V	olume	
9.73×10^{-3}	cubic meter, m ³	acre-inch	102.8
35.3	cubic meter, m ³	cubic foot, ft ³	2.83×10^{-2}
6.10×10^{4}	cubic meter, m ³	cubic inch, in ³	1.64×10^{-5}
2.84×10^{-2}			
	liter, L (10^{-3} m^3)	bushel, bu	35.24
1.057	liter, L (10^{-3} m^3)	quart (liquid), qt	0.946
3.53×10^{-2}	liter, L (10^{-3} m^3)	cubic foot, ft ³	28.3
0.265	liter, L (10^{-3} m^3)	gallon	3.78
33.78	liter, L (10^{-3} m^3)	ounce (fluid), oz	2.96×10^{-2}
2.11	liter, L (10^{-3} m^3)	pint (fluid), pt	0.473
	N.	Aass	
2.20×10^{-3}	gram, g (10^{-3} kg)	pound, lb	454
3.52×10^{-2}	gram, g (10^{-3} kg)	ounce (avdp), oz	28.4
2.205	kilogram, kg	pound, lb	0.454
0.01	kilogram, kg	quintal (metric), q	100
1.10×10^{-3}	kilogram, kg	ton (2000 lb), ton	907
1.102	megagram, Mg (tonne)	ton (U.S.), ton	0.907
1.102	tonne, t	ton (U.S.), ton	0.907
	Yield	and Rate	
0.893	kilogram per hectare, kg ha ⁻¹	pound per acre, lb acre ⁻¹	1.12
7.77×10^{-2}	kilogram per cubic meter, kg m ⁻³	pound per bushel, bu ⁻¹	12.87
1.49×10^{-2}	kilogram per hectare, kg ha ⁻¹	bushel per acre, 60 lb	67.19
1.59×10^{-2}	kilogram per hectare, kg ha ⁻¹	bushel per acre, 56 lb	62.71
1.86×10^{-2}	kilogram per hectare, kg ha ⁻¹	bushel per acre, 48 lb	53.75
0.107	liter per hectare, L ha ⁻¹	gallon per acre	9.35
893	tonnes per hectare, t ha ⁻¹	pound per acre, lb acre ⁻¹	1.12×10^{-3}
893	megagram per hectare, Mg ha ⁻¹	pound per acre, lb acre ⁻¹	1.12×10^{-3} 1.12×10^{-3}
0.446	megagram per hectare, Mg ha ⁻¹		
2.24	meter per second, m s ⁻¹	ton (2000 lb) per acre, ton acre ⁻¹ mile per hour	2.24 0.447
	C	Surface	
10	square meter per kilogram, m² kg ⁻¹	c Surface square centimeter per gram, cm ² g ⁻¹	0.1
1000	square meter per kilogram, m² kg ⁻¹	square millimeter per gram, mm ² g ⁻¹	0.001
	De	ensity	
1.00	megagram per cubic meter, Mg m ⁻³	gram per cubic centimeter, g cm ⁻³	1.00
	D	essure	
9.90	megapascal, MPa (10 ⁶ Pa)	atmosphere	0.101
10	megapascal, MPa (10 Pa)	bar	0.101
2.09×10^{-2}	pascal, Pa	pound per square foot, lb ft ⁻²	47.9
1.45×10^{-4}	pascal, Pa	pound per square inch, lb in ⁻²	6.90×10^3
			D OH X THE

(continued on next page)

Conversion Factors for SI and non-SI Units

o convert Column 1 into Column 2, multiply by	Column 1 SI Unit	Column 2 non-SI Unit	To convert Column into Column 1, multiply by
1.7.7	Tem	perature	
1.00 (K - 273)	Kelvin, K	Celsius, °C	1.00 (°C + 273)
$(9/5 ^{\circ}\text{C}) + 32$	Celsius, °C	Fahrenheit, °F	5/9 (°F - 32)
	Energy, Work	, Quantity of Heat	
9.52×10^{-4}	joule, J	British thermal unit, Btu	1.05×10^{3}
0.239	joule, J	calorie, cal	4.19
10^{7}	joule, J	erg	10^{-7}
0.735 2.387×10^{-5}	joule, J joule per square meter, J m ⁻²	foot-pound calorie per square centimeter (langley)	1.36 4.19×10^{4}
10 ⁵	newton, N	dyne	10^{-5}
1.43×10^{-3}	watt per square meter, W m ⁻²	calorie per square centimeter minute (irradiance), cal cm ⁻² min ⁻¹	698
	Transpiration	and Photosynthesis	
3.60×10^{-2}	milligram per square meter second, $mg m^{-2} s^{-1}$	gram per square decimeter hour, g dm ⁻² h ⁻¹	27.8
5.56×10^{-3}	milligram (H ₂ O) per square meter second, mg m ⁻² s ⁻¹	micromole (H ₂ O) per square centi- meter second, μmol cm ⁻² s ⁻¹	180
10^{-4}	milligram per square meter second, mg m ⁻² s ⁻¹	milligram per square centimeter second, mg cm ⁻² s ⁻¹	10^{4}
35.97	milligram per square meter second, mg m ⁻² s ⁻¹	milligram per square decimeter hour, mg dm ⁻² h ⁻¹	2.78×10^{-2}
7.T. O		ne Angle	1.75 10.2
57.3	radian, rad	degrees (angle), °	1.75×10^{-2}
		Electricity, and Magnetism	
$\frac{10}{10^4}$	siemen per meter, S m ⁻¹ tesla, T	millimho per centimeter, mmho cm ⁻¹ gauss, G	$0.1 \\ 10^{-4}$
		Measurement	
9.73×10^{-3}	cubic meter, m ³	acre-inches, acre-in	102.8
9.81×10^{-3} 4.40	cubic meter per hour, m ³ h ⁻¹ cubic meter per hour, m ³ h ⁻¹	cubic feet per second, ft ³ s ⁻¹ U.S. gallons per minute, gal min ⁻¹	101.9 0.227
8.11	hectare-meters, ha-m	acre-feet, acre-ft	0.123
97.28	hectare-meters, ha-m	acre-inches, acre-in	1.03×10^{-2}
8.1×10^{-2}	hectare-centimeters, ha-cm	acre-feet, acre-ft	12.33
	Conc	entrations	
1	centimole per kilogram, cmol kg-1	milliequivalents per 100 grams, meq 100 g ⁻¹	1
0.1	gram per kilogram, g kg-1	percent, %	10
1	milligram per kilogram, mg kg ⁻¹	parts per million, ppm	1
	Rad	ioactivity	
2.7×10^{-11}	becquerel, Bq	curie, Ci	3.7×10^{10}
2.7×10^{-2} 100	becquerel per kilogram, Bq kg ⁻¹ gray, Gy (absorbed dose)	picocurie per gram, pCi g ⁻¹ rad, rd	37 0.01
100	sievert, Sv (equivalent dose)	rem (roentgen equivalent man)	0.01
	Plant Nutr	ient Conversion	
2.20	Elemental	Oxide	0.405
2.29	P	P_2O_5	0.437
1.20 1.39	K Ca	K ₂ O CaO	0.830 0.715
1.66	Mg	MgO	0.602



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Division S-1—Soil Physics

- 1087–1094 Inspectional Analysis of Convective-Dispersion Equation and Application on Measured Breakthrough Curves. M.K. Shukla, F.J. Kastanek, and D.R. Nielsen
- 1095–1103 Determination of Preferential Flow Model Parameters. S.D. Logsdon
- 1104–1114 Analytical Models for Soil Pore-Size Distribution After Tillage. Feike J. Leij, Teamrat A. Ghezzehei, and Dani Or
- 1115–1126 Soil Consistence and Structure as Predictors of Water Retention. W.J. Rawls and Ya.A. Pachepsky
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- 1134–1142 Accounting for Soil Spatial Autocorrelation in the Design of Experimental Trials. M. Fagroud and M. Van Meirvenne
- 1143–1150 Models for Estimating Soil Particle-Size Distributions. Sang Il Hwang, Kwang Pyo Lee, Dong Soo Lee, and Susan E. Powers

Division S-1—Notes

1151–1158 Vertical Distributions of Carbon Dioxide Diffusion Coefficients and Production Rates in Forest Soils. Shoji Hashimoto and Masakazu Suzuki

Division S-2—Soil Chemistry

- 1159–1171 Structural Components of Humic Acids as Determined by Chemical Modifications and Carbon-13 NMR, Pyrolysis-, and Thermochemolysis-Gas Chromatography/Mass Spectrometry. Berny Chefetz, Myrna J. Salloum, Ashish P. Deshmukh, and Patrick G. Hatcher
- 1172–1181 Correlating Manganese X-Ray Absorption Near-Edge Structure Spectra with Extractable Soil Manganese. Christopher A. Guest, Darrell G. Schulze, Ian A. Thompson, and Don M. Huber
- 1182–1189 Soil Chemical Properties Controlling Zinc²⁺ Activity in 18 Colorado Soils. *Kathryn M. Catlett, Dean M. Heil, Willard L. Lindsay, and Michael H. Ebinger*
- 1190–1197 Effect of Carbonate on the Adsorption of Selenate and Sulfate on Goethite. *H. Wijnja and C.P. Schulthess*

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DIVISION S-1—SOIL PHYSICS

Inspectional Analysis of Convective-Dispersion Equation and Application on Measured Breakthrough Curves

M. K. Shukla,* F. J. Kastanek, and D. R. Nielsen

ABSTRACT

Several miscible displacement experiments were carried out in three 10-, 20-, and 30-cm mollisol and antisol filled soil columns. A strong linear relationship between pore-water velocity (ν) and apparent diffusion coefficient (D) was obtained for both soil columns $(r^2>0.92)$. We also derived the nondimensional laws for equilibrium adsorption convective-dispersion equation (CDE) using inspectional analysis, which reduced the physical constants and variables in CDE from seven to four nondimensional- π quantities. After scaling, the times of effluent arrival were nearly the same and all the breakthrough curves (BTCs) coalesced into a very narrow region of scaled time.

DIMENSIONAL AND INSPECTIONAL analysis are useful tools for determining the physically significant scale factors. The empirical scale factors can be obtained through functional normalization technique. Although scaling techniques can be applied in many ways, the principle remains the formulation of relevant equations with smallest possible number of variables from the known physical laws and boundary conditions (Simmons et al., 1979; Tillotson and Nielsen, 1984; Sposito and Jury, 1985; Shook et al., 1992).

During the past several decades, large numbers of miscible displacement experiments have been carried out in laboratory soil columns and in fields (Nielsen and Biggar, 1961; Krupp and Elrick, 1968; Gaudet et al., 1977; van Genuchten and Wierenga, 1977; van Gunachten et al., 1977; Rao et al., 1980; Nkedi-Kizza et al., 1984; Smettem, 1984; de Smedt and Wierenga, 1984; de Smedt et al., 1986; Selim et al., 1987; Seyfried and Rao, 1987; Li et al., 1994). Most of the above studies mainly concentrated on v > 0.1 cm h⁻¹. Few studies examine the variation of transport parameters across a wide range of

lengths, and soils. The linear relationship between ν and D in saturated soil columns has been reported by de Smedt and Wierenga (1984). We conducted 56 displacement experiments through 10-, 20-, and 30-cm loam and sandy loam soil columns. The purpose of this study was to reduce the one-dimensional CDE and the corresponding initial and boundary conditions to a few nondimensional- π terms by inspectional analysis. The second objective was to scale time of effluent arrival of measured BTCs using the nondimensional scale factors or π terms. The third objective was to derive relationships between ν and D from both loam and sandy loam soil columns.

 ν , from 0.02 to 2.6 cm h⁻¹ using different displacement

THEORY

Miscible Displacement Equation

Several appropriate one-dimensional miscible displacement equations solved for different boundary conditions have been used to describe the experimental observations of this laboratory study. They included convective-diffusion and mass transfer equations based on adsorbed solutes being in equilibrium and others not in equilibrium with the solid soil phase as well as the inclusion of two-site and mobile-immobile water assumptions. The applicability of such equations has been published elsewhere. For the purpose of this scaling study, we focus our attention on the one-dimensional equilibrium adsorption equation for conditions of steady water flow

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x}$$
 [1]

where R is the retardation factor, C is the solution concentration (M L⁻³); D is the apparent diffusion coefficient (L² T⁻¹), t is the time (T), v is the average pore-water velocity (L T⁻¹) and x is the distance from the inflow boundary in the direction of flow (L). For linear adsorption, $R = 1 + (\rho K_D) \theta^{-1}$ where ρ is the soil bulk density (M L⁻³), K_D is the distribution coefficient equal to S C^{-1} , S is the adsorbed concentration (M M⁻¹) and θ is the volumetric soil water content (L³ L⁻³).

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Abbreviations: BTC, breakthrough curve; CDE, convective-dispersion equation; *D*, apparent diffusion coefficient; *v*, pore-water velocity.

The initial and boundary conditions used for the solution of Eq. [1] are:

$$C = 0 x \ge 0 t = 0$$

$$\frac{\partial C}{\partial x} = 0 x \to \infty t > 0$$

$$C = C_0 x = 0 0 < t < t_0$$

$$C = 0 x = 0 t > t_0$$
[2]

where C_0 is the solute concentration at the inlet boundary. For the experimental results of this study, a constant flux boundary condition at the inlet provided nearly identical results.

The solution of Eq. [1] (Lapidus and Amundson, 1952) is

$$\frac{C(x,t)}{C_0} = 0.5 \operatorname{erfc} \left[\frac{Rx - vt}{\sqrt{4DRt}} \right]
- 0.5 \operatorname{exp} \left(\frac{vx}{D} \right) \operatorname{erfc} \left[\frac{Rx + v}{\sqrt{4DR}} \right]
+ 0.5 \operatorname{erfc} \left[\frac{Rx - v(t - t_0)}{\sqrt{4DR(t - t_0)}} \right]
- 0.5 \operatorname{exp} \left(\frac{vx}{D} \right) \operatorname{erfc} \left[\frac{Rx + v(t - t_0)}{\sqrt{4DR(t - t_0)}} \right].$$
[3]

For a continuous application of C_0 at the inlet $(t < t_0)$, the last two terms of Eq. [3] are ignored.

Scaling by Inspectional Analysis

Scale factors are simple conversion factors, which relate characteristics of one system to corresponding characteristics of another. Scale factors can be derived from different kinds of dimensional analyses. Here we use inspectional analysis to reduce the miscible displacement equations along with its corresponding initial and boundary conditions to a few nondimensional π terms while eliminating as many physical constants and variables as possible. The stepwise procedure for obtaining the nondimensional π terms is described by Hellums and Churchill (1961), and Tillotson and Nielsen (1984).

Note that the variables in Eq. [1] are C, x, and t and the parameters or physical constants are K_D , ρ , θ , D, ν , and C_0 . The variables are made nondimensional by dividing by arbitrary reference quantities C_0 , x_0 , and t_0 . Hence, substituting the non-dimensional variables ($C^* = C/C_0$, $x^* = x/x_0$, and $t^* = t/t_0$) into Eq. [1] and [2] yields

$$R\frac{\partial C^*}{\partial t^*} = \frac{Dt_0}{x_0^2} \frac{\partial^2 C^*}{\partial x^{*2}} - \frac{vt_0}{x_0} \frac{\partial C^*}{\partial x^*}$$
[4]

and the modified initial and boundary conditions

$$C^* = 0 x^* \ge 0 t^* = 0$$

$$\frac{\partial C^*}{\partial x^*} = 0 x^* \to \infty t^* > 0$$

$$C^* = 1 x^* = 0 0 < t^* < 1$$

$$C^* = 0 x^* = 0 t^* \ge 1$$
[5]

Equating the coefficients Dt_0/x_0^2 and vt_0/x_0 to unity, the values of t_0 and x_0 are obtained as follows.

$$\frac{Dt_0}{x_0^2} = 1 \Rightarrow \frac{Dt_0^2}{x_0^2t_0} = 1 \Rightarrow \frac{D}{v^2t_0} = 1 \text{ or } t_0 = \frac{D}{v^2}$$
 [6]

and

$$\frac{vt_0}{x_0} = 1 \Rightarrow \frac{vD}{x_0v^2} = 1 \Rightarrow \frac{D}{x_0v} = 1 \text{ or } x_0 = \frac{D}{v}$$
 [7]

Substituting Eq. [6] and [7] into Eq. [4] yields the nondimensional equation

$$R\frac{\partial C^*}{\partial t^*} = \frac{\partial^2 C^*}{\partial x^{*2}} - \frac{\partial C^*}{\partial x^*}$$
 [8]

which is identical to the classical dimensionless equation obtained when a Peclet number $P = vx_0/D$ has been substituted into Eq. [1]. From inspection of Eq. [8] and the initial and boundary conditions [5], it can be seen that C^* depends only on $t^* = t/t_0 = v^2t/D$, $x^* = x/x_0 = xv/D$, and R. The general form of Eq. [1] becomes

$$\pi_1 = G(\pi_2, \, \pi_3, \, \pi_4)$$
 [9]

where G is some function which exactly describes the interrelationship between the terms $\pi_1 = C/C_0$, $\pi_2 = v^2t/D$, $\pi_3 = xv/C_0$ D, and $\pi_4 = R$. From Eq. [9] it is can be inferred that whenever two or more soil systems have similar values for π_2 , π_3 , and π_4 , they will have similar solute concentration versus soil depth or time curves. The scale factors are obtained by equating corresponding π terms. From the original Eq. [1], it can be seen that C is dependent upon the six quantities -t, R, D, x, v, and C_0 . Equation [9] shows that nondimensional concentration is dependent on three quantities— π_2 , π_3 , and π_4 —a result in direct agreement with the Buckingham Pi theorem. The four nondimensional quantities were reduced to four linear equations by taking the logrithm of both sides of the π terms. The coefficient matrix for the parameters and variables in four nondimensional groups was obtained in the same manner as Shook et al. (1992). The rank of the coefficient matrix, obtained through elementary column operations (Rawlings, 1988), was four, which was equal to the number of nondimensional scaling factors.

MATERIALS AND METHODS

Two soils—a loam and a sandy loam—were selected for experimentation. The loam, identified as an Entisol, was collected from the 0- to 15-cm depth from the Farmers Training Center at Pyhra, Lower Austria, and the sandy loam, identified as a Mollisol, was collected from the 40- to 70-cm depth from the experimental farm of the University of Agricultural Sciences, Vienna located at GrossEnzersdorf, near Vienna. The loam had an average particle diameter, *d*, of 0.0158 mm and that of the sandy loam was 0.0508 mm. The separate portions of each of the air-dried soils that passed through a 2-mm sieve were prepared into laboratory soil columns and also analyzed for their physical and chemical properties. Soil was packed into 10-cm i.d. acrylic plastic cylinders having lengths of 10, 20, and 30 cm. Care was taken to follow exactly the same

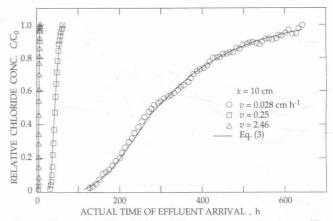


Fig. 1. Observed and fitted Cl breakthrough curves using the equilibrium convective-dispersion equation for a slow, medium, and fast pore-water velocity through a 10-cm loam soil column.

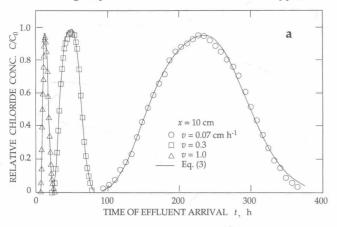
procedure for packing all of the soil columns. The porosity and bulk density were quantitatively determined for each soil column. Each soil column was slowly saturated from the bottom with 0.1 M CaBr₂. The steady-state flow required for obtaining a given pore-water velocity was adjusted by measuring the effluent volume with respect to time. The effluent solutions were collected at fixed time intervals in small plastic bottles. Displacement experiments using MgCl₂ for several different pore-water velocities were performed on each column starting with the lowest pore-water velocity. For a step input, the displacing solution was switched back to the connate solution when no more connate ions were detected in the effluent (Fig. 1). For a pulse input, ~300 mL of displacing solution was followed by the connate solution (Fig. 2). All the experiments were conducted at a temperature controlled to 20 ± 2°C. Concentrations of Cl⁻ and Br⁻ were determined by titration. An accurate value of soil water content for each soil column was determined gravimetrically at the cessation of each experiment. Fifty-six displacement experiments were conducted using 13 different soil columns. A more elaborate description of the experimental details is available (Shukla, 1998; Shukla et al., 2000).

RESULTS

Analysis of Measured Chloride Breakthrough Curves

Mass Recoveries

The amount of Cl pulse applied was independent of column length, pore-water velocities, and soil type; and



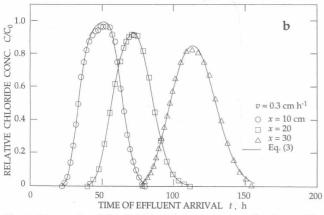


Fig. 2. Observed and fitted Cl breakthrough curves using the equilibrium convective-dispersion equation (a) for a slow, medium, and fast pore-water velocity in 10-cm loam soil columns, and (b) from 10-, 20-, and 30-cm loam soil columns for a pore-water velocity of 0.3 cm h⁻¹.

was ~300 mL. The concentration versus time BTCs showed the progressive attenuation of the initial concentration when 300 mL of solute was displaced through greater macroscopic lengths (Fig. 2b). The mass recoveries from both loam and sandy loam soil columns were very high (always >97% of the applied pulse of solute). The experiments for very slow water velocities in loam soil columns for both solute boundary conditions (step and pulse) showed early arrival of Cl in the effluent solution and long flat BTCs (Shukla et al., 2000). These experiments illustrated the contribution of molecular diffusion in the transport process. A detailed theoretical analysis of each experiment and the measured BTC is presented in Shukla et al. (2000).

Parameter Estimation

Measured Cl concentrations in the effluent for each of the 56 experiments plotted as a function of time were fitted to Eq. [3] using program CFITIM (van Genuchten, 1981) to ascertain the values of D and the retardation factor, R. These values together with measured values of soil bulk density (ρ), soil water content (θ), and average v are given in Table 1 for a step solute input into two 10-cm long columns of loam for a range of v from 0.025 to 2.60 cm h $^{-1}$. For this range of v, values of D increase approximately one order of magnitude while values of R manifest a slight increasing trend with a mean of 1.05. As illustrated in Fig. 1 for the smallest, intermediate, and largest values of v for Column 2, each of the 17 experimental BTCs were nicely described by Eq. [3] using the values given in Table 1.

Measured and calculated terms for pulse solute inputs into 10-, 20-, and 30-cm columns of the loam and sandy loam soils are given in Tables 2 and 3, respectively. In

Table 1. Soil column data with parameters of Eq. [1] for a step solute input into 10-cm columns of loam soil.

Exp. no.†	Col no.‡	ρ§	$\theta \P$	v#	$D^{\dagger\dagger}$	R‡‡
		g cm ⁻³	${ m cm^3~cm^{-3}}$	cm h ⁻¹	$cm^2 h^{-1}$	
1	1	1.433	0.438	0.025	0.028	0.902
2	2	1.413	0.447	0.028	0.035	0.919
3	1	1.433	0.438	0.056	0.027	0.905
4	2	1.413	0.445	0.051	0.026	0.867
5	2	1.413	0.448	0.074	0.025	0.867
6	1	1.433	0.438	0.11	0.026	1.125
7	2	1.413	0.447	0.12	0.030	0.930
8	1	1.433	0.440	0.18	0.042	1.040
9	2	1.413	0.447	0.25	0.042	1.085
10	2	1.413	0.445	0.50	0.069	1.081
11	1	1.433	0.441	0.51	0.073	1.169
12	1	1.433	0.440	0.72	0.103	1.200
13	2	1.413	0.447	0.77	0.104	1.067
14	2	1.413	0.448	1.32	0.176	1.126
15	1	1.433	0.440	1.39	0.207	1.190
16	2	1.413	0.477	2.47	0.353	1.155
17	1	1.433	0.440	2.60	0.333	1.203
mean		1.422	0.444			1.049

[†] Exp. No. = experiment number.

[‡] Col. = column.

 $[\]S \rho = \text{soil bulk density.}$

 $[\]P \theta$ = pore water velocity.

[#] v =water velocity

 $[\]dagger\dagger D =$ Apparent diffusion coefficient.

 $[\]ddagger R = Retardation factor.$

Table 2. Soil column data with parameters of Eq. [1] for a pulse solute input into 10-, 20-, and 30-cm columns of loam soil.

Exp. no.†	Col no.‡	ρ§	$\theta \P$	v#	$D^{\dagger\dagger}$	$R^{\ddagger\ddagger}$
		${\rm g}~{\rm cm}^{-3}$	$\mathrm{cm^3~cm^{-3}}$	$cm h^{-1}$	$cm^2 h^{-1}$	
			m column			
18	3	1.480	0.437	0.07	0.020	1.07
19	3	1.480	0.438	0.10	0.025	1.00
20	3 3	1.480	0.438	0.30	0.048	1.00
21	3	1.480	0.437	0.50	0.071	1.09
22	3	1.480	0.438	0.70	0.100	1.08
23	3	1.480	0.438	1.00	0.208	1.03
mean		1.480	0.438			1.05
		20-с	m column			
24	4	1.458	0.425	0.07	0.025	0.93
25	4	1.458	0.426	0.10	0.031	1.02
26	4	1.458	0.425	0.30	0.067	1.01
27	4	1.458	0.425	0.50	0.100	1.02
28	4	1.458	0.427	0.70	0.140	1.04
29	4	1.458	0.426	1.00	0.217	1.07
mean		1.458	0.426			1.02
		30-с	m column			
30	5	1.482	0.405	0.02	0.022	0.85
31	5	1.482	0.405	0.05	0.022	0.84
32	6	1.454	0.414	0.07	0.027	0.96
33	6	1.454	0.414	0.10	0.033	0.97
34	7	1.490	0.407	0.30	0.075	0.96
35	7	1.490	0.407	0.50	0.107	0.99
mean		1.475	0.409			0.93

[†] Exp. No. = experiment number.

Table 3. Soil column data with parameters of Eq. [1] for a pulse solute input into 10-, 20-, and 30-cm columns of sandy loam soil.

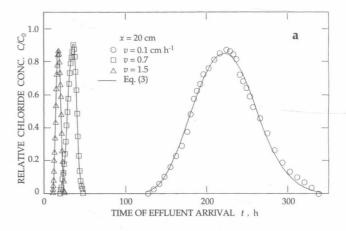
Exp. no.†	Col no.‡	ρ§	θ¶	v#	$D^{\dagger\dagger}$	$R^{\ddagger\ddagger}$
	7.	g cm ⁻³	cm³ cm ⁻³	cm h ⁻¹	$cm^2 h^{-1}$	
		10-c	m columns			
36	8	1.450	0.429	0.10	0.023	1.20
37	8	1.450	0.428	0.32	0.025	1.10
38	8	1.450	0.428	0.48	0.056	1.10
39	9	1.510	0.420	0.68	0.061	1.04
40	9	1.510	0.422	1.01	0.111	1.13
41	9	1.510	0.420	1.50	0.200	1.11
42	9	1.510	0.420	1.99	0.250	1.12
mean		1.484	0.424			1.11
		20-c	m columns			
43	10	1.433	0.431	0.10	0.026	0.94
44	10	1.433	0.430	0.29	0.048	1.00
45	10	1.433	0.430	0.53	0.074	1.05
46	10	1.433	0.430	0.72	0.106	1.02
47	11	1.460	0.429	1.00d	0.204	1.05
48	11	1.460	0.430	1.47	0.341	1.03
49	11	1.460	0.429	1.96	0.404	1.06
mean		1.446	0.430			1.02
		30-с	m columns			
50	12	1.484	0.415	0.11	0.027	1.06
51	12	1.484	0.420	0.32	0.052	1.03
52	12	1.484	0.415	0.50	0.082	1.03
53	12	1.484	0.415	0.70	0.127	1.08
54	13	1.468	0.417	1.02	0.214	1.07
55	13	1.468	0.417	1.50	0.378	1.06
56	13	1.468	0.420	1.93	0.465	1.09
mean		1.477	0.417		3.100	1.06

Exp. No. = experiment number. Col. = column.

Table 2, it is evident that the bulk densities of the columns were slightly larger than those in Table 1 yielding slightly smaller corresponding soil water contents. On the other hand, values of R are near unity and not consistently related to either ν or ρ . In all cases, theoretical curves matched the experimental results—Fig. 2a shows BTCs for three velocities for a 10-cm column of loam while Fig. 2b shows BTCs for a velocity of 0.3 cm h⁻¹ for three column lengths. The information in Table 3 regarding the sandy loam is similar—values of D are related to v, and slight deviations of soil water content and retardation factor are generally, but not consistently related to soil bulk density. For all sandy loam columns, theoretical curves matched the experimental results— Fig. 3a shows BTCs for three velocities for a 20-cm column of sandy loam while Fig. 3b shows BTCs for a velocity of 0.3 cm h⁻¹ for the three column lengths of 10, 20, and 30 cm.

Relations Between Apparent Diffusion Coefficient and Pore-water Velocity

Within the range of average pore-water velocities studied, molecular diffusion dominates the dispersion of the



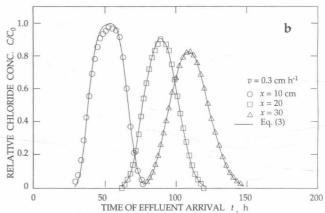


Fig. 3. Observed and fitted Cl breakthrough curves using the equilibrium convective dispersion equation (a) for a slow, medium, and fast pore-water velocity in 20-cm loam soil columns, and (b) from 10-, 20-, and 30-cm sandy loam soil columns for a pore-water velocity of 0.3 cm h^{-1} .

[±] Col. = column.

 $[\]S \rho = \text{soil bulk density.}$

 $[\]P \theta$ = pore water velocity.

[#]v = water velocity

 $[\]dagger\dagger D = Apparent diffusion coefficient.$

 $[\]ddagger \ddagger R = Retardation factor.$

⁼ soil bulk density.

pore water velocity.

water velocity

Apparent diffusion coefficient.

 $[\]ddagger R = Retardation factor.$

Table 4. Parameters for the linear regression of D versus v for the loam and sandy loam soil columns.

Soil	Length	Intercept	Slope	R^2	n
		Step-solute input			
Loam	10	0.016	0.128	0.99	17
		Pulse-solute input			
Loam	10	-0.004	0.185	0.92	6
	20	-0.007	0.201	0.99	6
	30	0.015	0.187	0.99	6
Sandy loam	10	-0.013	0.132	0.99	7
Sundy Tourn	20	-0.018	0.218	0.98	7
	30	-0.024	0.248	0.99	7

Cl at smaller displacement velocities and gives way to convective dispersion at greater velocities. Hence, for relatively small average pore-water velocities we expect D to have values close to that of the diffusion coefficient of Cl, D_o , in the soil solution, and to be only somewhat dependent of v. At relatively larger velocities, D should be strongly related to v. The results in Table 4 are consistent with those expectations. Linear regressions between D and v derived from the 56 experiments summarized in Table 4 are all highly significant with values of R^2 ranging between 0.92 and 0.99. However, not shown in Table 4 for the smaller velocities when diffusion dominates, the regression between D and v using the five values of v < 0.075 cm h^{-1} (Table 1) was not significant $(R^2 = 0.49)$.

The relations between D/D_0 and Peclet number (vd/D_0) given as solid lines in Fig. 4 satisfy the equation

$$\frac{D}{D_o} = 1 + m \left(\frac{vd}{D_o} \right)^n \tag{10}$$

where the value of $D_{\rm o}$ is estimated from $D_{\rm o}=0.660 D_{\rm m}$ with $D_{\rm m}$ being the Cl diffusion coefficient for free solution (2.15 \times 10⁻⁵ cm² s⁻¹). The results from the seven loam columns and the six sandy loam columns of this study fall between the earlier reported values derived from measurements made in a natural undisturbed field soil by Biggar and Nielsen (1976) and for laboratory

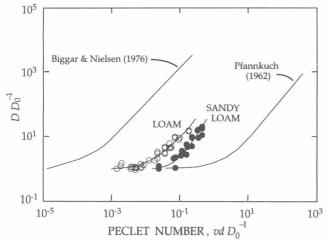
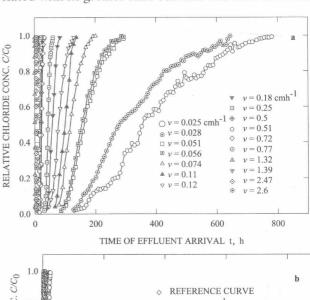


Fig. 4. The relationship between DD_0^{-1} and Peclet Number.

Table 5. Parameters for Eq. [10] for the results illustrated in Fig. 4.

Soil	m	n	d	D_{0}
			mm	cm ² h ⁻¹
Laboratory columns				
Pfannkuch (1962)	0.5	1.20	0.156	0.0220
Sandy loam	70.5	1.71	0.0508	0.0216
Loam	141	1.21	0.0158	0.0222
Field soil	17780	1.11	0.00272	0.0250
Biggar and Nielsen (1976)				

columns of graded sands and other single-grained materials reported by Pfannkuch (1962). Here, we estimated the values of D_0 for the loam and the sandy loam to be 0.0222 and 0.0216 cm² h⁻¹, respectively, using the average value of θ measured for the 35 and 21 experiments of each soil, respectively. In Table 5, it can be seen that values of m increase with decreasing values of average particle diameter, d, while values of n range between 1 and 2. In the loam and sandy loam soils as well as the field soil, decreasing average particle diameter (increasing clay content) is associated with soil structure. The loam has relatively large pores as a result of microaggregates, and the sandy loam, although containing less clay than the loam, nevertheless has large pores also associated with its microaggregates as well as those associated with its greater sand content. The field soil mani-



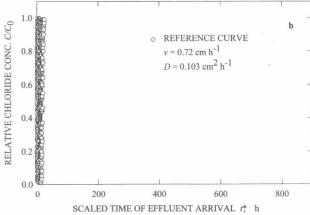


Fig. 5. Measured Cl breakthrough curves in 10-cm loam soil columns for step Cl application (a) theoretical and (b) scaled.

fests the greatest value of m because of its large poresize distribution owing to its high clay content, its aggregation, and its natural field structure.

Scaling of Measured Chloride Breakthrough Curves

Having obtained the parameters (Tables 1–3) of the theoretical BTCs that adequately describe the measured BTCs, nondimensional- π terms from Eq. [1] were ascertained. Compared with the impact of the large range of pore-water velocities on the positions of the BTCs, we ignore the small variations of retardation factor, R, and consider its value constant for the scaling process. By taking advantage of the strong linear relationships between D and v given in Table 4, the π_2 term which contains the time of effluent arrival can be used for scaling the BTCs. Scale factors were obtained for a given displacement length by equating the corresponding π_2 terms of each BTC with that of an arbitrary reference curve. For the reference curve for each displacement length, we selected the BTC having a pore-water velocity near the mean pore-water velocity for which displacements were made. From the scale factors the scaled time of effluent arrival was calculated for each BTC.

Measured and scaled BTCs with respect to the time of effluent arrival from the 10-cm columns of loam leached

a 1.0 x = 10 cmRELATIVE CHLORIDE CONC. C/C $v = 0.07 \text{ cm h}^{-1}$ v = 0.1v = 0.3v = 0.5 $\nabla v = 0.7$ 0.6 v = 1.00 200 300 400 TIME OF EFFLUENT ARRIVAL 1.0

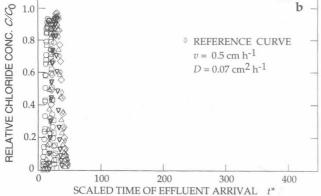
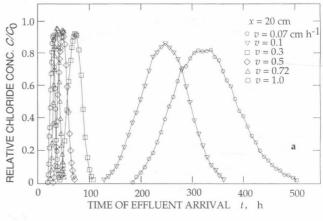


Fig. 6. Measured Cl breakthrough curves in 10-cm loam soil columns for pulse Cl application (a) theoretical and (b) scaled.

with a step input of Cl are presented in Fig. 5 for the 17 different pore-water velocities. Depending on the pore-water velocity, the times required to measure the entire BTC ranged from as few as 6 h to as many as 780 h. After scaling, the times of arrival are nearly the same for all curves with the 17 BTCs coalesced into a very narrow region of scaled time. From these data using only one soil length, the scaling procedure appears to be reasonably successful.

Displacing a pulse input of Cl at different pore-water velocities through progressively longer columns of the loam provides a more critical examination of the scaling process. In Fig. 6a, we note that each BTC reaches about the same relative maximum for each of the values of ν and that all seven curves are coalesced nicely in Fig. 6b. These results appear equivalent and consistent with those in Fig. 5 when a step input of Cl was diplaced through the same length column (10 cm). However, in Fig. 7 and 8, the effectiveness of the scaling procedure appears less satisfactory. It is apparent that the relative maximum Cl concentration begins to decrease with decreasing values of ν for the 20-cm long columns, and is especially noticeable for the 30-cm columns.

The results of displacing a pulse input of Cl at different pore-water velocities through progressively longer columns of the less structured sandy loam appear more



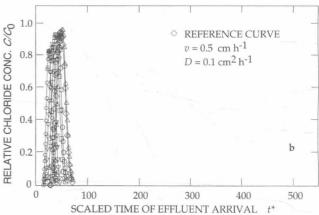


Fig. 7. Measured Cl breakthrough curves in 20-cm loam soil columns for pulse Cl application (a) theoretical and (b) scaled.

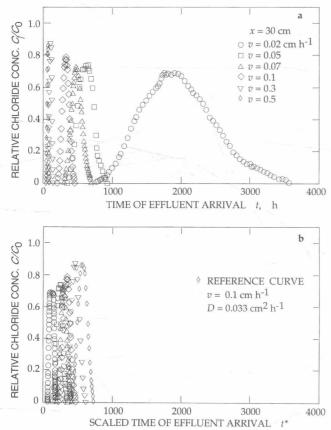


Fig. 8. Measured Cl breakthrough curves in 30-cm loam soil columns for pulse Cl application (a) theoretical and (b) scaled.

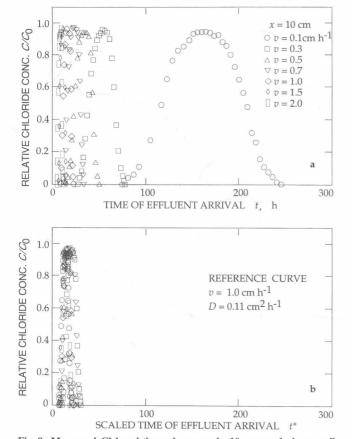
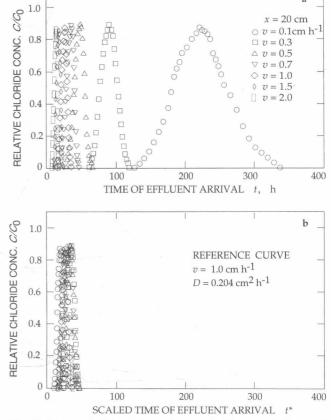


Fig. 9. Measured Cl breakthrough curves in 10-cm sandy loam soil columns for pulse Cl application (a) theoretical and (b) scaled.



x = 20 cm

1.0

Fig. 10. Measured CI breakthrough curves in 20-cm sandy loam soil columns for pulse Cl application (a) theoretical and (b) scaled.

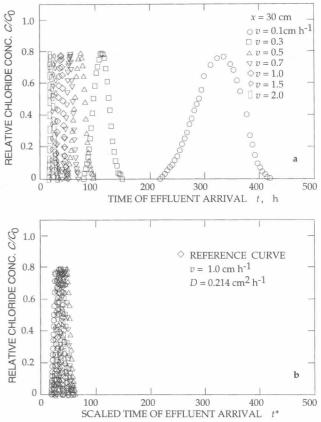


Fig. 11. Measured CI breakthrough curves in 30-cm sandy loam soil columns for pulse Cl application (a) theoretical and (b) scaled.

consistent with the proposed scaling process. In Fig. 9, 10, and 11, we note for each soil length that each BTC reaches about the same relative maximum for each of the values of ν and that all seven curves are coalesced to about the same degree. Regardless of the magnitude of ν , for each column length, the relative maximum Cl concentration is constant (\sim 0.95, 0.9, and 0.8 for x=10,20, and 30 cm, respectively).

CONCLUSIONS

The equilibrium CDE fitted BTCs matched the measured BTCs very well (r^2 always > 0.97). The retardation coefficient remained independent of ν , ρ , θ , and soil type and remained close to one. The D remained less dependent on ν for lower average pore-water velocities and for relatively larger velocities, D increased linearly with v for both the soils. The nondimensional quantities obtained by inspectional analysis reduced the number of independent variables in CDE from seven to four. The scale factors obtained from π_2 terms reduced the times of effluent arrival and the measured BTCs were coalesced into a very small region of scaled time. In general, the proposed scaling process appeared more consistant for BTCs from less structured sandy loam soil columns. The relative maximum Cl concentration was also constant for these sandy loam columns regardless of the magnitude of pore-water velocity.

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Determination of Preferential Flow Model Parameters

S. D. Logsdon*

ABSTRACT

Solute transport models that include a preferential flow component require many input parameters. There are well established procedures to determine micropore parameters, but procedures to determine macropore parameters are not well established. The objective of this paper was to evaluate methods to independently measure macropore parameters. The test model used was MACRO, a transient-state, twoflow domain model. The key macropore parameters in the model are saturated and boundary hydraulic conductivities (K, and Kh), the absolute value of the boundary head between macropore and micropore domains (h_b) , the exponent (n^*) of the relation between K(variables are defined in the appendix) and water content (θ) , the macropore fraction (θ_{sma}), and the half spacing (d) between equivalent parallel fractures. As an example this study used soils in the Des Moines lobe (Mollisols with textures ranging from sandy loam to silty clay). Data used to calculate model parameters included wet-end K- θ -h and K(h), and results from image analysis. For the MACRO model, the parameters fit the equations best when h_b was assumed to be 30 mm. For the measured data with assumed $h_b = 30$ mm, n^* had a median of 2.1 and a range from 0 to 5.2, median K_b was 15 mm h^{-1} with a range from 1 to 100 mm h^{-1} , and the median K_s was 122 mm h^{-1} with a range from 7 to 741 mm h^{-1} . The calculated d ranged from 1 to 847 mm, and θ_{sma} ranged from 0.001 to 0.053 m³ m⁻³. Depending on the data available, the various techniques can be used to determine input parameters for preferential flow models.

Preferential flow can result in rapid movement of surface-applied solute through the soil (Germann et al., 1984; Quisenberry et al., 1994). Many preferential flow models have been developed in recent years to enhance the accuracy of predicted solute transport. The addition of preferential flow mechanisms into models require additional inputs that are difficult to obtain. Independent measurements are the most appropriate way to determine the necessary input parameters models (Beven, 1991; Dane and Moltz, 1991; Grayson et al., 1992). Well-established procedures are available to determine input parameters for the micropore domain, but standard procedures have not yet been established for macropore input parameters.

Currently a number of techniques are used to estimate macropore properties (Edwards et al., 1993; McCoy et al., 1994). Techniques have been developed to describe the macropore region in the soil, including infiltration under negative head (Ankeny et al., 1988; Perroux and White, 1988), desorption at the wet-end (McCoy, 1989; Logsdon et al., 1993), image analysis (Protz et al., 1987; Edwards et al., 1988; Moran et al., 1989; Logsdon et al., 1990; Thompson et al., 1992), and multiple-tracer techniques (Jaynes et al., 1995). Measuring soil hydraulic and physical properties for the macropore region should not be an end in itself. Such information should

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be used for input in preferential flow models, and to test the assumptions of the models. The objectives of this paper were to evaluate methods to independently measure or calculate macropore parameters, and to use this information to test the assumptions of the preferential flow model MACRO.

THEORY MACRO Model

The MACRO model has been parameterized and compared with data for numerous laboratory and field scales (Jarvis et al., 1991; Jabro et al., 1994; Saxena et al., 1994; Larsson and Jarvis, 1999a). The following equations relating to the key macropore parameters of the MACRO model are discussed in Jarvis and Larsson (2001) and Larsson and Jarvis (1999a). The soil is divided into macropore and micropore flow domains. Between the two domains there are boundary values for hydraulic conductivity, absolute value of head, and water content (K_b , h_b , and θ_b). Within the macropore domain, the relation between h and θ is assumed to be

$$h = h_b \left[(\theta_s - \theta) / (\theta_s - \theta_b) \right]$$
 [1]

where h_b is boundary head, θ is the water content (L³ L⁻³) when $\theta > \theta_b$, and θ_s is the saturated water content. The difference, $\theta_s - \theta_b$, is also called the macropore fraction (θ_{sma}), and is influenced by shrinking and swelling (not shown). Hydraulic conductivity is assumed to be related to θ as

$$(K - K_b)/(K_s - K_b) = [(\theta - \theta_b)/(\theta_s - \theta_b)]^{n*}$$
 [2]

where K is the hydraulic conductivity (L T⁻¹) for $\theta > \theta_b$, K_b is the boundary hydraulic conductivity, and n^* is an empirical exponent. Water and solute exchange between micropore and macropore domains are inversely related to the square of d, the equivalent half spacing of parallel fractures. Since θ_{sma} is contributed by hexagonal fracture patterns, biopores, and interpedal voids, as well as parallel fractures, the calculated d is an equivalent fracture spacing.

Literature Parameterization for MACRO Model

Those who have run the MACRO model needed to determine model input parameters. Usually the $\theta_{\rm s}$ was measured, and the $\theta_{\rm b}$ was measured for an assumed or calibrated $h_{\rm b}$ value. Saxena et al. (1994) measured the soil water retention curve for the micropore region, and the smallest h was 100 mm. For one soil, they set the $h_{\rm b}$ at 100 or 150 mm for different depths, but they calibrated $h_{\rm b}$ for the other soil, ending up with $h_{\rm b} = 500$ mm. Jabro et al. (1994) also measured the soil water retention curve, and the smallest h was 100 mm. They set the $h_{\rm b}$ at 400 mm by defining macropores as those pores smaller than 75 μ m. Larsson and Jarvis (1999a,b) assumed $h_{\rm b} = 100$ mm, and measured the corresponding θ from tension table measurements.

Since θ_{sma} is the difference between θ_s and θ_b , the range of values can be compared. Jabro et al. (1994) had θ_{sma} values ranging from 0.01 to 0.08 m³ m⁻³. Saxena et al. (1994) had θ_{sma} values ranging from 0.02 to 0.13 m³ m⁻³. Larsson and Jarvis (1999a) measured θ_{sma} ranging from 0.02 to 0.07 m³ m⁻³. Based on a different data set (but the same soil), they adjusted