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The Feasibility of Shallow Time Domain Reflectometry Probes to Describe Solute Transport Through Undisturbed Soil Cores

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ABSTRACT

Rapid and nondestructive methods for determining solute transport properties are useful in many soil science applications. Recently, a series of field methods and a time domain reflectometry (TDR) method that could estimate some of the mobile-immobile model (MIM) parameters, immobile water content (θ_{im}) and mass exchange coefficient (α), have been reported. The first objective of this study was to determine an additional parameter, dispersion coefficient (D_m), using the TDR method. The three MIM parameters were estimated from the TDR-measured data, and the estimated parameters were compared with the estimated parameters from the effluent data. The second objective was to determine whether the TDR-determined parameters from the surface 2-cm soil layer could be used to predict effluent breakthrough curves (BTC) at the 20-cm depth. The TDR-determined parameters were used to calculate effluent BTCs using the CXTFIT computer program. Parameters obtained by curve fitting of the three parameters simultaneously using TDR data were not similar to the parameters obtained from the effluent BTCs. The parameter estimations were improved by fixing one or two independently determined parameter(s) before curve fitting for the remaining unknown parameter(s). The calculated BTCs were similar to the observed BTCs with coefficient of determination (r^2) being 0.99 and root mean square error (RMSE) being 0.036. The TDR data obtained from shallow soil layers were successfully used to describe solute transport through undisturbed soil cores.

Many studies (Rao et al., 1980; Nkedi-Kizza et al., 1983; Lee et al., 2000b) have shown that the MIM can describe some forms of preferential solute transport. The MIM includes three significant model parameters, immobile water content (θ_{im}), mass exchange coefficient (α), and dispersion coefficient (D_m), to describe nonsorbing, conservative solute transport. However, determining the three parameters is not easy, especially in the field.

So far, methods have been developed to estimate only some of the parameters. Clothier et al. (1992) first introduced a method to estimate θ_{im} of field soil using a tension infiltrometer and a conservative tracer (Br^-). The Br^- tracer was applied through a tension infiltrometer with steady-state infiltration. After applying sufficient infiltration of tracer, soil samples were taken and analyzed to calculate θ_{im}. If all of the soil water is mobile, the concentration of the tracer should equal the input concentration. Based on the concentration difference between the input solution and the soil solution, one can calculate θ_{im}. Similarly, Jaynes et al. (1995) presented a technique that could estimate both θ_{im} and α. They developed a log-linear equation using the MIM. The equation represented a relationship between resident tracer concentration and time of tracer application and could be used to estimate both θ_{im} and α. To apply the method, a sequence of benzoate tracers (ST) were applied through a tension infiltrometer. The Jaynes et al. (1995) ST method was tested in the field (Casey et al., 1997) and in the laboratory (Lee et al., 2000b). Casey et al. (1997) and Lee et al. (2000b) reported that the ST method provided MIM parameters representative of the soil.

Based on the ST method, Lee et al. (2000a) recently presented a TDR method that could simultaneously estimate θ_{im} and α. The method used a shallow TDR probe installed into a surface 2-cm soil layer to measure resident concentration changes as a function of time following a surface infiltration of $CaCl_2$ solution. They analyzed the TDR measurements to estimate θ_{im} and α using a log-linear relationship derived from the ST method. The TDR method provided an extensive number of data points whereas the ST method provided a limited number of data points depending on availability of the sequential tracers. Lee et al. (2000a) reported that the estimates of θ_{im} and α from the TDR method were very similar to the estimates obtained from inverse curve fitting of the effluent breakthrough curve (BTC) data. Although one can estimate θ_{im} and α in the field using one of the methods described above, the dispersion coefficient, D_m, is not estimated. Dispersion of solute is a primary mechanism for solute transport in soil. Thus, it would be useful to estimate D_m along with θ_{im} and α.

Furthermore, the structure of a shallow soil layer may or may not be similar to that of deeper soil. Steenhuis et al. (1999) presented a conceptual model in which a layer near the surface became saturated and distributed the water and solutes to the preferential flow paths. In the conceptual model, movement of water and solute in the layer (so-called distribution layer) was different than that below the distribution layer. It is important to examine whether solute transport properties obtained from the shallow soil layer (0–2 cm) using the TDR method can be used to characterize solute transport deeper in the soil.

The first objective of this study was to determine D_m, in addition to θ_{im} and α, using the shallow TDR method. The MIM parameters obtained from TDR were com-

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Abbreviations: BTC, breakthrough curves; CI, confidence interval; LLT, log-linear TDR; MIM, mobile-imobile model; RMSE, root mean square error; ST, sequence of benzoate tracers; TDR, time domain reflectometry.

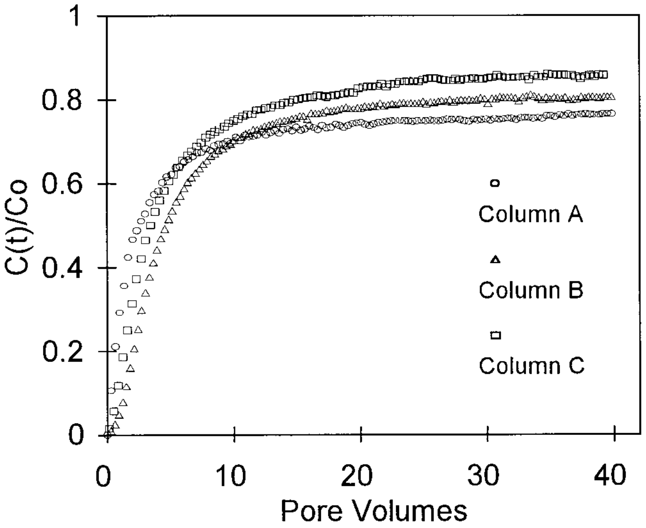

Fig. 1. The relative resident conentrations, $C(t)/C_0$, obtained from the shallow (0- to 2-cm soil layer) time domain reflectometry probe for three soil columns. The *x*-axis is based on the 2-cm sampling layer.

pared with the parameters estimated from the observed effluent BTCs for the same soil cores. The second objective was to test whether the three parameters obtained from the shallow (0–2 cm) soil layer could be used to predict effluent BTCs at a deeper depth, 20 cm. The TDR determined parameters were used in a simulation study to predict effluent BTCs for comparison with the observed effluent BTCs. The second objective is an approach to evaluate not only parameters individually but to evaluate the usefulness of the set of parameters to predict solute behavior.

MATERIALS AND METHODS

Parameter Determination

Data from Lee et al. (2000a) were used in this study. Briefly, Lee et al. (2000a) used three 20-cm long by 12-cm diam. undisturbed saturated soil cores. The soil was Nicollet silt loam (fine-loamy, mixed, superactive, mesic Aquic Hapludolls). A two-rod, 2-mm diam. and 80-mm long TDR probe was installed diagonally from the surface to a depth of 2 cm. Soil disturbance was minimized by installing the TDR probe diagonally instead of horizontally. Lee et al. (2000a) assumed that the TDR probe measured the average bulk soil electrical conductivity of the top 2-cm layer of soil. In this paper, the dispersion coefficient, D_m, in addition to θ_{im} and α, was estimated using the data from the TDR method (Lee et al., 2000a). Inverse curve fitting with the CXTFIT (Toride et al., 1999) program of the resident concentration BTCs from the TDR method was done. The depth for the curve fitting in CXTFIT was set at 1 cm, which was the average depth of the sampling volume (0–2 cm) of the TDR probe. The collected effluent samples of $CaCl_2$ were also analyzed to determine the three parameters using CXTFIT. The TDR determined parameters were compared with the parameters estimated from curve fitting the effluent data.

Predicting Effluent Breakthrough Curves

A computer simulation study was conducted to study the feasibility of using the estimated MIM parameters obtained from TDR to predict solute transport through the soil columns. TDR data from the surface 2-cm soil layer were used to determine MIM parameters which were used to predict effluent BTCs for the 20-cm soil columns. The simulation study focuses on use of the combined parameters to predict solute transport in contrast to the direct comparison of parameters which focuses on individual comparison of the parameters. By comparing the TDR-derived predicted BTCs with the observed BTCs, we have some insight into the practical usefulness of the parameters obtained from the TDR technique.

The MIM analytical solutions from CXTFIT were used to calculate effluent BTCs. The predicted BTCs were generated using MIM parameters estimated from the TDR method. These calculated BTCs were compared with the observed effluent BTC. Two quantitative measures, coefficient of determination (r^2) and RMSE (Snedecor and Cochran,1967; Willmott et al., 1985), were used to evaluate the predicted BTCs.

RESULTS AND DISCUSSION

Figure 1 shows the relative resident concentration values, $C(t)/C_o$, obtained from TDR for 0- to 2-cm soil layer. The resident concentrations increased relatively quickly at the beginning of the tracer application and increased relatively slowly over the remaining application period. Conceptually, because the initial mobile water (or active flow pathways) was first replaced with the input tracer solution mainly by convection, the resident concentration increased relatively quickly at the beginning of the experiment. As the mobile domain was replaced with input tracer, tracer in the mobile domain

Table 1. Comparison of parameter estimates from the TDR method and from the effluent data.

			TDR		
		Effluent	**3-fit**	**Clothier θ_{im}-fixed**	**Lee α, θ_{im}-fixed**
Column A	θ_{im}/θ	0.39 ± 0.02	0.15 ± 0.03	0.24†	0.31 ± 0.01‡
	α, h^{-1}	0.02 ± 0.006	0.001 ± 0.001	0.01 ± 0.003	0.01 ± 0.001‡
	D_m, $cm^2\ h^{-1}$	100 ± 15.2	182 ± 32.2	176 ± 14.1	82 ± 19.6
Column B	θ_{im}/θ	0.28 ± 0.01	0.17 ± 0.02	0.20†	0.32 ± 0.01‡
	α, h^{-1}	0.01 ± 0.004	0.001 ± 0.001	0.001 ± 0.007	0.03 ± 0.001‡
	D_m, $cm^2\ h^{-1}$	102 ± 5.8	275 ± 36.2	256 ± 22.8	151 ± 28.6
Column C	θ_{im}/θ	0.35 ± 0.01	0.13 ± 0.02	0.14†	0.30 ± 0.01‡
	α, h^{-1}	0.07 ± 0.008	0.002 ± 0.002	0.003 ± 0.001	0.04 ± 0.001‡
	D_m, $cm^2\ h^{-1}$	141 ± 6.8	278 ± 25.9	268 ± 17.9	129 ± 24.9

† Parameters are determined using the Clothier et al. (1992) method.
‡ Parameters are determined using the log-linear TDR (Lee et al., 2000a) method.

diffused over time into the immobile water domain (or relatively nonactive flow pathways). The diffusion process was relatively slow compared with the convection process.

The relative resident concentrations from the soil extracts ranged from 0.76 to 0.86 after applying 40 pore volumes of input solution. Because the relative resident concentrations from the soil extracts were less than one, some of the water-filled pore spaces were not replaced with input solution, indicating the presence of an immobile water domain. Thus, incorrectly assuming complete replacement of the soil water with input solution after 40 pore volumes of application would result in a 14 to 24% error in maximum relative resident concentration.

Comparison of the Parameter Values from the TDR Method and from the Effluent Data

The estimated MIM parameters from the effluent data and from the TDR method for the three soil columns are shown in Table 1. The estimates marked "3-fit" are obtained from curve fitting of TDR-measured resident concentrations. The 95% confidence intervals (CI) from CXTFIT are reported as well. The estimated immobile water fractions (θ_{im}/θ) obtained from the TDR method were lower than the θ_{im}/θ from the effluent data. The means of θ_{im}/θ from the TDR method and from the effluent data were 0.15 and 0.34, respectively. The estimated α values from the TDR method were lower than the estimates from the effluent data. The means of α (h^{-1}) from the TDR method and from the effluent data were 0.001 and 0.03, respectively. The means of D_m ($cm^2\ h^{-1}$) from the TDR method and from the effluent data were 223 and 114, respectively. For all three soil columns, the parameter estimates from the TDR method were not similar to the parameter estimates from the effluent data.

Note that the $C(t)/C_o$ values from the TDR method were from the surface 2-cm soil layer where the analytical solution in CXTFIT was sensitive to the surface boundary condition. Hence, small experimental errors leading to slight changes in the measurements in the surface 2-cm soil layer could cause relatively large deviations of fitted parameters. In this case, it would be desirable to estimate one or two of the parameter(s) and fix the parameter(s) before using inverse curve fitting to determine the remaining unknown parameter(s). By fixing θ_{im} or α, the inverse curve fitting could be used to solve for only one or two parameter(s) rather than for all three parameters. Thus, for each soil core, θ_{im} was estimated using Clothier et al. (1992) method. Immobile water content was determined based on the resident concentrations of the soil samples taken after infiltrating $CaCl_2$ solution (Clothier et al., 1992). The θ_{im} was then fixed during the inverse curve fitting of the TDR data to determine α and D_m. Similarly, θ_{im} and α were estimated using the Lee et al. (2000a) log-linear TDR method (LLT method) so that the two parameters could be fixed for the inverse curve fitting of the TDR data. Note that both the Clothier et al. (1992) and Lee et al. (2000a) methods did not require any additional experiments or sampling. Both methods used the data obtained from the shallow TDR method. Table 1 shows the Clothier and LLT determined θ_{im} or α values along with other estimated parameters. In the "Clothier θ_{im}-fixed" column, the θ_{im}/θ estimates from the Clothier et al. (1992) method were not within the 95% CI of the θ_{im}/θ estimates from the effluent data. The estimated α and D_m by fixing the separately determined θ_{im}/θ were also not similar to the estimates from the effluent data. In the "Lee α, θ_{im}-fixed" column, the θ_{im}/θ and α estimates from the LLT method were similar to the estimates from the observed effluent data although the CIs did not encompass each other. The D_m estimates obtained after fixing both θ_{im}/θ and α were similar to the estimates obtained from observed effluent data. Overall, the pa-

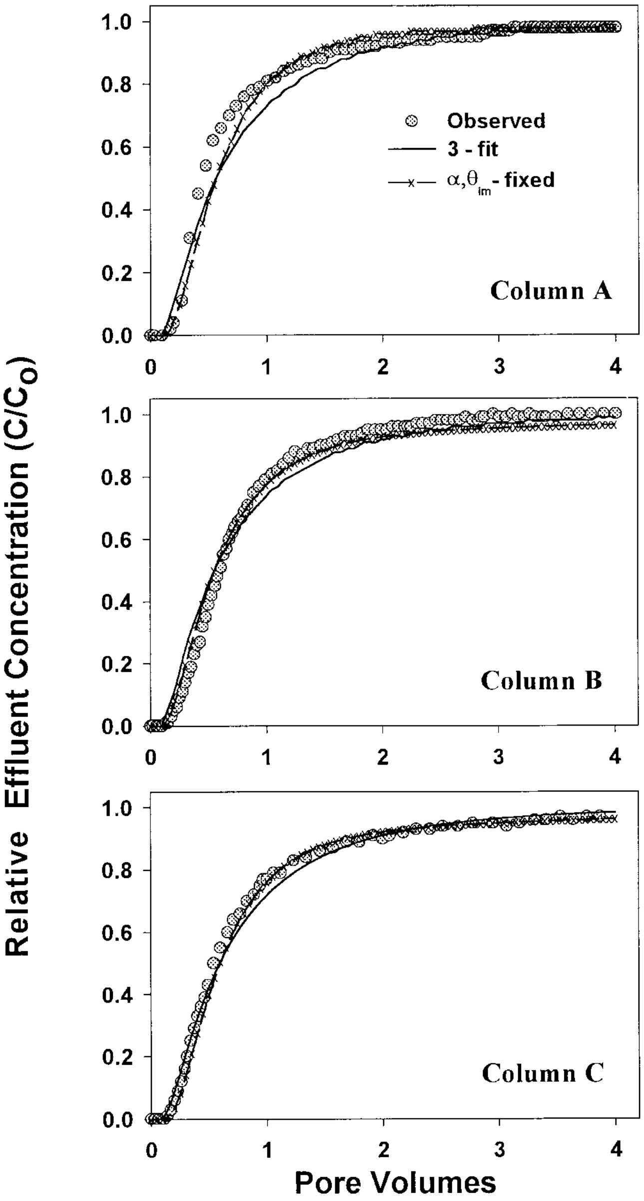

Fig. 2. The predicted effluent breakthrough curves (BTCs) are plotted along the observed BTCs for the three soil columns. The predicted BTCs are generated using the estimated parameters shown in Table 1. Analytical solutions of the mobile–immobile model from CXTFIT are used to calculate the effluent BTCs.

Table 2. Coefficient of determination, r^2, and root mean square error (RMSE) for the effluent fitted and the calculated breakthrough curves (BTC).

		Column A	Column B	Column C	Average
Effluent fitted	r^2	0.992	0.999	0.999	0.997
	RMSE	0.013 (1.0)†	0.009 (1.0)	0.006 (1.0)	0.009 (1.0)
3-fit	r^2	0.978	0.984	0.988	0.983
	RMSE	0.046 (3.5)	0.047 (5.2)	0.028 (4.7)	0.041 (4.6)
Clothier θ_{im}-fixed	r^2	0.981	0.985	0.987	0.984
	RMSE	0.038 (2.9)	0.046 (5.1)	0.027 (4.5)	0.037 (4.1)
Lee α, θ_{im}-fixed	r^2	0.993	0.995	0.998	0.995
	RMSE	0.034 (2.6)	0.035 (3.9)	0.019 (3.2)	0.029 (3.2)

† The ratios of the calculated RMSE to the RMSE from the fitted effluent data.

rameter estimates obtained by "Lee α, θ_{im}-fixed" seemed the most representative of effluent-determined parameters.

Comparison of the Predicted and Observed Breakthrough Curves

To test whether the information from the shallow soil could be used to predict chemical transport in the whole soil column, the set of TDR determined parameters from the surface 2-cm soil layer (Table 1) were used to predict effluent BTCs at the 20-cm depth. The predicted BTCs were generated using the analytical solution of MIM from the CXTFIT. The results of predicting BTCs are shown in Fig. 2 along with measured BTCs. The BTC marked "3-fit" used α, θ_{im}, and D_m values obtained from fitting three parameters simultaneously. The BTC marked "α, θ_{im}fixed" used the MIM parameters in the "Lee α, θ_{im}-fixed" column in Table 1. The predicted BTCs using parameters in the "Clothier θ_{im}-fixed" column in Table 1 were very similar to the predicted BTCs marked "3-fit". For clarity, "Clothier θ_{im}-fixed" BTCs are not shown in Fig. 2. For all three soil cores, the calculated BTCs were similar to the observed effluent BTCs. Table 2 shows the values of r^2 and RMSE to evaluate the accuracy of the inverse curve fitting and the predictions in describing the observed effluent BTCs. Coefficient of determination was computed for the nonlinear relationship based on Snedecor and Cochran (1967). The r^2 values for the effluent fitted and predicted BTCs ranged from 0.98 to 0.99 indicating the accuracy of the inverse curve fitting and predictions. RMSE for both the effluent fitted BTCs and the calculated BTCs are shown in Table 2. The average RMSEs for the effluent fitted BTCs were lower than those for the calculated BTCs. The average RMSEs for the effluent fitted and calculated BTCs were 0.009 and 0.036, respectively. The ratios of the predicted BTCs to the observed BTCs for RMSE were also calculated (Table 2). The average RMSE ratio of "3-fit", "Clothier θ_{im}-fixed", and "Lee α, θ_{im}-fixed" predicted BTCs to observed BTCs were 4.6, 4.1, and 3.2, respectively. The results implied that the parameter estimates obtained from fixing one or two parameters made better predictions of effluent BTCs than did the 3-fit estimates. The predictions were the best when "Lee α, θ_{im}-fixed" parameters were used.

Lee et al. (2000b) observed both resident concentrations and effluent data for a set of soil columns. They tested the MIM by evaluating the model's success in predicting resident tracer concentrations from parameters fitted to effluent BTCs and vice versa. They reported that predicting effluent data using resident concentrations seemed to work better than predicting resident concentrations using effluent data. We again note that the predicted effluent BTCs were obtained from the surface 2-cm soil layer and resident concentrations, whereas the measured effluent BTCs represented 20-cm long soil columns. In spite of these differences, the calculated effluent BTCs from the TDR method were very similar to observed effluent BTCs. These are promising results indicating the capability of the shallow TDR method to provide solute transport parameters that can be used to extrapolate chemical movement in deeper soil.

CONCLUSIONS

A simple TDR method designed to estimate θ_{im} and α was further evaluated for determining dispersion coefficient, D_m, in addition to θ_{im} and α. For the inverse curve fitting of the three MIM parameters, fixing one or two parameters improved estimation of dispersion coefficient. A simulation study showed that the parameters obtained from the shallow (0–2 cm) soil layer were successful in predicting effluent BTCs at the 20-cm depth. The TDR method was relatively simple. The TDR method required only a surface soil sample with minimum disturbance of soil, after applying a step input of salt solution. This shallow TDR method is a promising method and should be further examined in situ to delineate solute transport.

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DIVISION S-1—NOTES

A MODIFIED UPWARD INFILTRATION METHOD FOR CHARACTERIZING SOIL HYDRAULIC PROPERTIES

M. H. Young*, A. Karagunduz, J. Šimůnek, and K. D. Pennell

Abstract

This note describes a modified upward infiltration method (UIM), which combines laboratory experiments and inverse parameter estimation for determining soil hydraulic properties in the wetting direction. The laboratory method used a Mariotte system to impose a constant head boundary condition on the bottom of a soil column, allowing water to be taken up by the soil material under negative pressure head. Tensiometers installed along the column measured the change in soil pressure head before and after wetting front arrival. The HYDRUS-1D code was used to obtain an optimal set of van Genuchten parameters, using pressure head and cumulative flux data as auxiliary variables in the objective function. Two soil types (a fine sand and a sandy loam) were tested in triplicate in uniformly-packed soil columns. The results of the uniform column experiments were repeatable, and showed excellent fits between observed and predicted data. Fitted parameters were used in forward simulations to independently predict water flow behavior in layered columns of the same soil material. The forward simulations successfully predicted water flow for sand-over-loam and loam-over-sand combinations in layered columns. The relative simplicity of the experimental procedure and the availability of appropriate numerical models renders the modified upward infiltration method an alternative for determining wetting hydraulic properties of soils.

The measurement of soil hydraulic properties, specifically soil water content (θ)—soil water pressure head (ψ) and hydraulic conductivity (K)—water content (θ) functions, is needed to predict the direction and rate of water movement in unsaturated soils. However, the paired values of $\theta(\psi)$ and $K(\theta)$ are dependent upon the direction of wetting or drying (Dane and Wierenga, 1975; Hillel, 1998). Experimentation required to establish the functions in wetting and drying directions, and their intermediate values, often require specialized laboratory setups, which is why often times only the drying functions are determined (Hillel, 1998).

In the past few decades, several transient methods have been proposed for characterizing soil hydraulic properties, including one-step outflow (Parker et al., 1985), multi-step outflow (Eching and Hopmans, 1993; van Dam et al., 1994), and evaporation (Wind, 1968; Šimůnek et al., 1998a). Each of these methods use the change in column weight to infer changes in soil water content, and with the exception of Parker et al. (1985) and van Dam et al. (1994), either one or more tensiometers placed along the column to measure change in soil water potential. A review of inverse estimation of hydraulic properties was done by Hopmans and Šimůnek (1999).

Experimental methods have been shown to work for a variety of soil textures undergoing drying. However, they do not yield hydraulic properties for soils undergoing wetting, and the transfer of drying curves to wetting curves is not trivial. The UIM is one of a few methods capable of obtaining wetting properties of soils. The UIM was originally described by Hudson et al. (1996), who showed that the method was robust for uniform, sandy-textured soil samples. Wyckoff (1997) applied the method to a variety of clayey-textured soils, including those with swelling clays. Both studies used constant flux bottom boundary conditions, which reduces the usefulness of the flux as an optimization parameter because the flux is independent of the soil properties (Šimůnek and van Genuchten, 1997).

Other researchers have used variations of the UIM. For example, Karkare and Fort (1993) and Demond et al. (1994) used standard Tempe cells, and reversed the gradient in a series of equilibrium pressure steps, so that test solution in a graduated burette would be taken up spontaneously into the soil. In these cases, soil water pressure head was not measured, so gradients could have existed in the column at the end of the step, yielding noncorresponding values of θ (inside the column) and ψ (at the bottom boundary).

Controlling water intake by setting the bottom boundary pressure, coupled with intensive soil data collection could improve on these methods. Recently, Šimůnek et al. (2000) suggested using a tension-based UIM for

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Abbreviations: UIM, upward infiltration method.