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DEVELOPMENTS IN VADOSE ZONE SOIL SOLUTION EXTRACTION

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ABSTRACT

The study of water migration and contaminant transport in soils is of fundamental importance in hydrologic science. Movement of agrochemicals (nitrates, atrazine) and industrial solvents (TCE, carbontetrachloride) to the groundwater is of great public concern. In order for these chemicals to reach the groundwater, they must pass through the vadose zone. Thus, in order to predict travel times of contaminants toward the groundwater or to understand the underlying transport process, we need to characterize and sample the unsaturated zone. The need for an economical, readily available monitoring system with a broad range of applications is required by the practicing groundwater scientist and vadose zone hydrologist, given the growing recognition of the interdependence of the unsaturated zone and saturated zone processes. At present, there are few, if any, cost effective and practical field monitoring devices which incorporate the sophisticated sampling and data acquisition array necessary for representative monitoring of the vadose zone.

As concern for a save environment and groundwater quality increases, the importance of an accurate soil hydraulic description of the combined unsaturated-saturated porous system is increasingly recognized in the fields of environmental engineering and groundwater hydrology. With this wider interest, the spatial scale of interest has shifted to dimensions as large as a watershed, and to depths from the rooting zone to the groundwater. This trend in increasing larger spatial scales of the vadose zone brings along with it the presence of increasing soil heterogeneity within the considered system.

Therefore, methodologies need to be developed that allow for a rapid and accurate characterization for the soil hydraulic properties and its spatial variability.

The objectives of the WRC-sponsered research was to develop a single sampling unit which can be used to sample soil solution, but at the same time monitors continuously the soil water potential. The second objective was to demonstrate the potential application of this combined tensiometer-soil soluton extraction probe to estimate in situ the soil water retention and unsaturated hydraulic conductivity functions.

Keywords: Soils, Unsaturated Flow, Soil Moisture, Contaminant Transport, Water Quality Monitoring

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PROBLEM AND RESEARCH OBJECTIVES

Contamination of the subsurface due to point and non-point sources of pollution remains one of the most perplexing environmental issues of our time. There is growing awareness that gradual but pervasive deterioration of groundwater quality occurs by both point and non-point sources of contamination from agricultural and urban land uses. However, cause and effect relationships between these land uses and subsurface water quality remain partly an enigma.

For solutes to reach the groundwater, they must pass through the unsaturated soil or vadose region. Transport prediction requires accurate characterization of the soil and soil water environment, including hydraulic properties. The measurement of representative soil water pressure and soil solution concentrations is a fundamental task for the vadose zone hydrologist. The requirement for adherence to reproducible sample and data collection protocol is well known and understood by the increasing use and sophistication of numerical models. Interpretation of results can only be as meaningful as the manner in which the basic field data or samples are collected.

A sensor is proposed which allows measurement of soil water pressure and the sampling of soil water concurrently. The soil water energy status or soil water pressure can be measured by tensiometers. The technique of soil solution extraction utilizes identical porous ceramic cups as tensiometers. Various porous ceramic cup solution sampler designs have been described over the years, such as porous tube device, vacuum extractor, tension and suction lysimeter, soil water sampler, and porous ceramic sampler.

Although there is an increasing need for improved in-situ soil solution samplers, developments in this area are rather scarce (Essert and Hopmans, 1997).

Currently, many laboratory and field methods exist to determine the highly nonlinear soil hydraulic functions, represented by the soil water retention and unsaturated hydraulic conductivity curves. Most methods require restrictive initial and boundary conditions, which make measurements time-consuming, range-restrictive and expensive. The inverse problem of parameter identification for distributed numerical models has been applied in groundwater hydrology and field petroleum engineering since the early seventies. Its application to the vadose zone started later, and has been mostly limited to parameter estimation of soil hydraulic properties. The parameter estimation technique as defined in this study involves the indirect estimation of soil hydraulic functions by numerical solution of the governing flow equation, and comparison of the numerical solution with experimental data. In this procedure, an analytical model with yet unknown parameter values describes soil hydraulic properties. An experiment is setup under controlled conditions with prescribed initial and boundary conditions. During the experiment one or more flow-controlled variables are measured. Subsequently, the Richards equation is solved numerically using the parameterized hydraulic functions with initial estimates for their parameters. These parameters are optimized by minimization of an objective function containing the sums of squared deviations between observed and predicted flow variables, using repeated numerical simulations of the flow process.

The first objective of this investigation was to develop a simple single probe, which allows soil solution sampling during or between soil water pressure measurements. The proposed segmented tensiometer-solution sampling probe minimizes soil disturbance by integrating the two units into a single probe. We report on the design and operation of an easy-to-assemble unit consisting of two compartments, with the objective to measure soil water pressure at a single depth only, and which can be used simultaneously for soil water sampling near the tensiometric measurement location. The second objective of this study was to demonstrate the potential application of in-situ soil water extraction using combined soil water pressure and solution extraction measurements to estimate soil water retention and unsaturated hydraulic conductivity parameters.

REVIEW OF METHODOLOGY

Combined Probe

Conventional tensiometers and soil solution samplers are very similar in design, and consist of a porous ceramic cup glued into a PVC pipe. The tensiometer is filled with water, installed into the soil to the desired depth, and soil water pressure is monitored using a pressure transducer after pressure equilibration. Simply by extending sampling tubing from the porous cup chamber to a sampling bottle, the same design is used as a soil solution sampling probe. After soil installation, a sample bottle is attached to the sampling tube and vacuum is applied to the solution sampler. Sampling duration depends on soil type, soil water pressure, applied vacuum, and required sample volume. Simultaneous measurement of soil water pressure and soil solution extraction either requires installation of two separate probes, or repeated filling and draining of the tensiometer housing.

Construction of the proposed combined tension-solution probe requires two separate porous ceramic compartments within a 2.2 cm OD PVC pipe, of variable length. For the design in Fig. 1, a 5.4 cm long porous 2.2 cm OD ceramic cup was cut in half. An acrylic barrier in which two holes were drilled to accommodate small diameter tubing separated the two compartments of the porous ceramic cup. Two holes were drilled near the top end of the PVC pipe. The small diameter tubing is guided through the holes at the top of the PVC pipe and through the acrylic barrier into the bottom compartment of the probe. One tube feeds just through the barrier while the other tube extends to the bottom of the porous ceramic cup. The longer sampling tube at the base of the ceramic cup is used for the transfer of soil solution from the ceramic cup to the sample bottle by vacuum application. The shorter vent tube near the acrylic barrier allows for air entry into the solution sampling compartment as it is emptied. Also, a positive pressure can be applied to the vent tube thereby assisting in the transfer of solution from the sampling compartment to the sample bottle above ground. The two-compartment ceramic cup assembly was cemented to the bottom of the PVC pipe. A short piece of 1.6 cm OD acrylic tubing was cemented into the top of the tensiometer compartment, and closed with a rubber septum. Thus, the combined probe consists of two separate compartments, with the top compartment acting as a tensiometer, whereas the bottom chamber serves as the soil water extraction device (Figure. 1).

Column experiments were carried out to evaluate the performance of the combined tensiometer-solution sampling probe and to compare data with those collected with conventional tensiometers and suction solution samplers. The experiment consisted of three columns packed with Hanford sandy loam, Panoche loam and Yolo silt loam. Soils were leached with a saturated solution of calcium sulfate to prevent dispersion of soil aggregates. Subsequently, all soils were air-dried, sieved through a 2-mm screen, and packed to a depth of 11.0 cm in the 20.7 cm diameter columns. The soil columns were

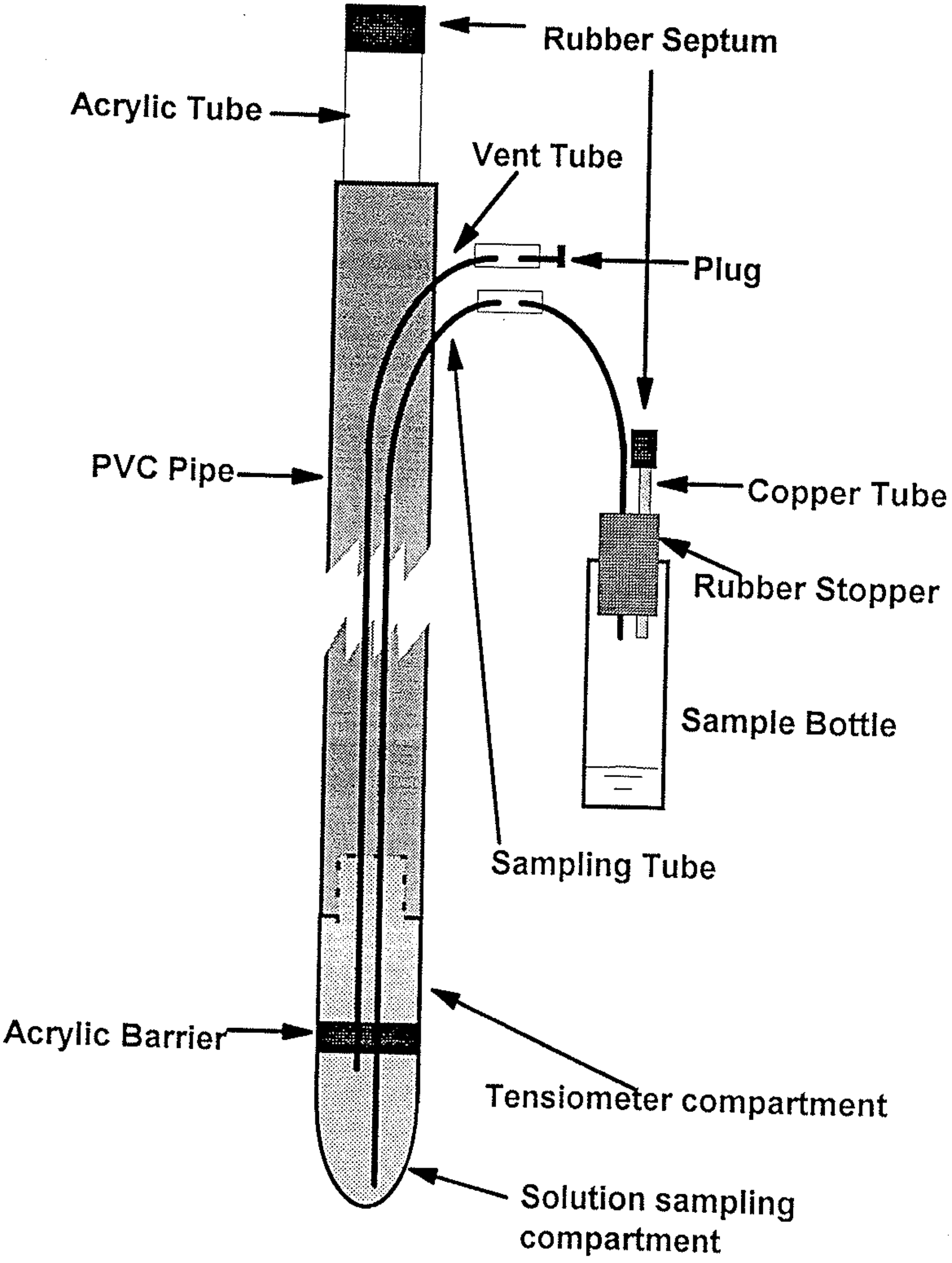

Figure 1. Design of combined tension-soil solution probe.

subsequently saturated with a 97.0 meq L^{-1} $CaCl_2$ (stock solution) by immersion in a solution bath and were placed on a tension table. Each column was instrumented with two conventional suction solution samplers, one conventional tensiometer, and a single combined tensiometer-solution sampling probe. The columns were drained by applying suction (expressed in equivalent height of water) steps of 30 cm, 100 cm, 200 cm, 300 cm and 400 cm to the burette. Changes in soil water pressure were monitored with the tensiometers and the combined probes. Soil solution was extracted (vacuum was 50 cm greater than the applied suction) after the measured soil water pressure was equal to the suction applied to the soil columns.

Multi-step soil water extraction

Water Flow Theory and Parameter optimization

The concept of the proposed method is based on the premise that the soil's hydraulic properties can be estimated from the measurement of extracted soil water volume and soil water potential values at various locations as a function of time. Applying a number of vacuum increments to a ceramic soil water extraction device does this. Although the experiments will occur in three dimensions, we will assume axial symmetry, which reduces the Richards' equation to two dimensions, which for an isotropic rigid porous media can be written as

$$\frac{\partial \theta}{\partial t}=\frac{1}{r}\frac{\partial}{\partial r}\left(rK\frac{\partial h}{\partial r}\right)+\frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z}\right)+\frac{\partial K}{\partial z} \quad , (1)$$

where r is the radial coordinate [L], z is the vertical coordinate positive upward [L], and t is time [T]. The time-derivative term on the left is determined by the slope of the soil water retention curve, $\theta(h)$, whereas the unsaturated hydraulic conductivity K [LT^{-1}] is a function of the soil matric potential h [L]. Boundary and initial conditions for which (1) was solved is dependent on the specific experiment, but can be generally defined as

$$h(r,z,t) = h_i(z) \qquad t = t_0 \qquad 0 < r < R \tag{2}$$

$$h(r,z,t) = h_{lb} \qquad z = \text{-55cm} \quad 0 < r < R \qquad t_0 < t < t_{end} \tag{3}$$

$$h(r,z,t) = h_{ex} \qquad r = r_i \text{ (2.70 cm)} \qquad -11.5 < z < -8.5 \text{ cm} \tag{4}$$

$$q(r,z,t) = 0 \qquad \text{remaining boundaries} \qquad t_0 < t < t_{end} \tag{5}$$

where $r = R$ denotes the radius of the flow domain [L], the coordinate $z = 0$ is placed at the top of the flow domain, t_0 and t_{end} correspond to the beginning and end of the extraction experiment [T], respectively, and r_i is the inside radius of the extraction device [L]. In solving Eq. (1), subject to conditions (2) through (5), the unsaturated hydraulic properties are defined by

$$S_e = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \frac{1}{(1+|\alpha h^n|)^m} \tag{6}$$

and

$$K(\theta) = K_s S_e^{1/2}\left[1-\left(1-S_e^{1/m}\right)^m\right]^2 \qquad h<0 \tag{7}$$

$$K(\theta)=K_s \qquad h\geq 0 \qquad (8)$$

In expressions (6) through (8), S_e is the effective saturation [-], θ_r and θ_s denote the residual and saturated volumetric water contents [-], respectively; α [L^{-1}] and n [-] (m=1-1/n) are empirical parameters, and K_s is a fitted saturated hydraulic conductivity [LT^{-1}].

Parameters in (6) through (8) were estimated from maximization of the log-likelihood function, which includes differences between observed and predicted flow variables (Levenberg-Marquardt method). Assuming measurement errors to be independent with zero mean, the parameter optimization procedure is equivalent to minimization of a weighted least squares problem, which is cast in an objective function, OF($\boldsymbol{b}$), with $\boldsymbol{b}$ denoting the vector containing the optimized parameters:

$$\mathrm{OF}(\boldsymbol{b})=\sum_{j=1}^{m}\left(w_j\sum_{i=1}^{n_j}w_{i,j}\left[q_j^*(t_i)-q_j(t_i,\boldsymbol{b})\right]^2\right) \qquad (9)$$

where j represents the different sets of measurements (cumulative extraction volume, matric potential head at different locations, or water volume in flow domain), n_j is the number of measurements within a particular set, $q_j^*(t_i)$ are measurements of type j at time t_i, $q_j(t_i, \boldsymbol{b})$ are the corresponding model predictions using the parameters in $\boldsymbol{b}$, and w_j and $w_{i,j}$ are weighting factors associated with data type and data point, respectively. Assuming that measurement errors for all pressure transducers were identical, $w_{i,j}$ was set equal to one for all pressure measurements, whereas the water volume measurements were given a weighting factor value equal to 10. It here suffices to state that the Levenberg-Marquardt method is a standard method in nonlinear least-squares fitting, which in addition to the sum of squared residuals of (9) also provides confidence intervals for the optimized parameters. Additional details about the procedure can be found in Inoue et al. (1997).

Field experiment

A detailed overview of the field experiment is presented in Figure 2. The field soil is a Yolo silt loam with approximate clay content of 22 percent. Soil was excavated to a depth of 60 cm and leveled. A stainless steel square infiltrometer with sides of 1.2 m was pushed 10 cm in the soil. The ceramic extraction device was installed in the center of the plot (r = 0) with the center of the ceramic ring at z = -10 cm depth. Tensiometers were installed at the following positions: r = 4.0 cm and z = -10 cm (T_1); r = 6.0 cm and z = -15 cm (T_2); and r = 20.0 cm and z = -40 cm (T_3), and at r = 20 cm and z = -55 cm (T_4). The soil water potential measurements of this 55 cm deep tensiometer were fitted to a power function, which was used as lower boundary condition for the simulation model ($h = h_{lb}$). Vacuum was applied to the burette using a vacuum tank, which was evacuated, at a pre-determined vacuum for each of the solution extraction step increments. The plot was covered with a shelter to minimize temperature fluctuations, which would influence vacuum in the tank.

The 1.2 m square plot was ponded with a constant head of 0.5 cm water for about 3 days until the steady state infiltration rate was 1 cm h^{-1}. Subsequently, a plastic sheet to prevent soil evaporation covered the plot. The soil was allowed to drain for a period of 46.5 h at which time the total head gradient was about 0.3 cm cm^{-1}. After the 46.5 h of free drainage, the first vacuum extraction step was applied (h_{ex} = -195 cm for $46.5 < t < 71.2$ h). Subsequent vacuum

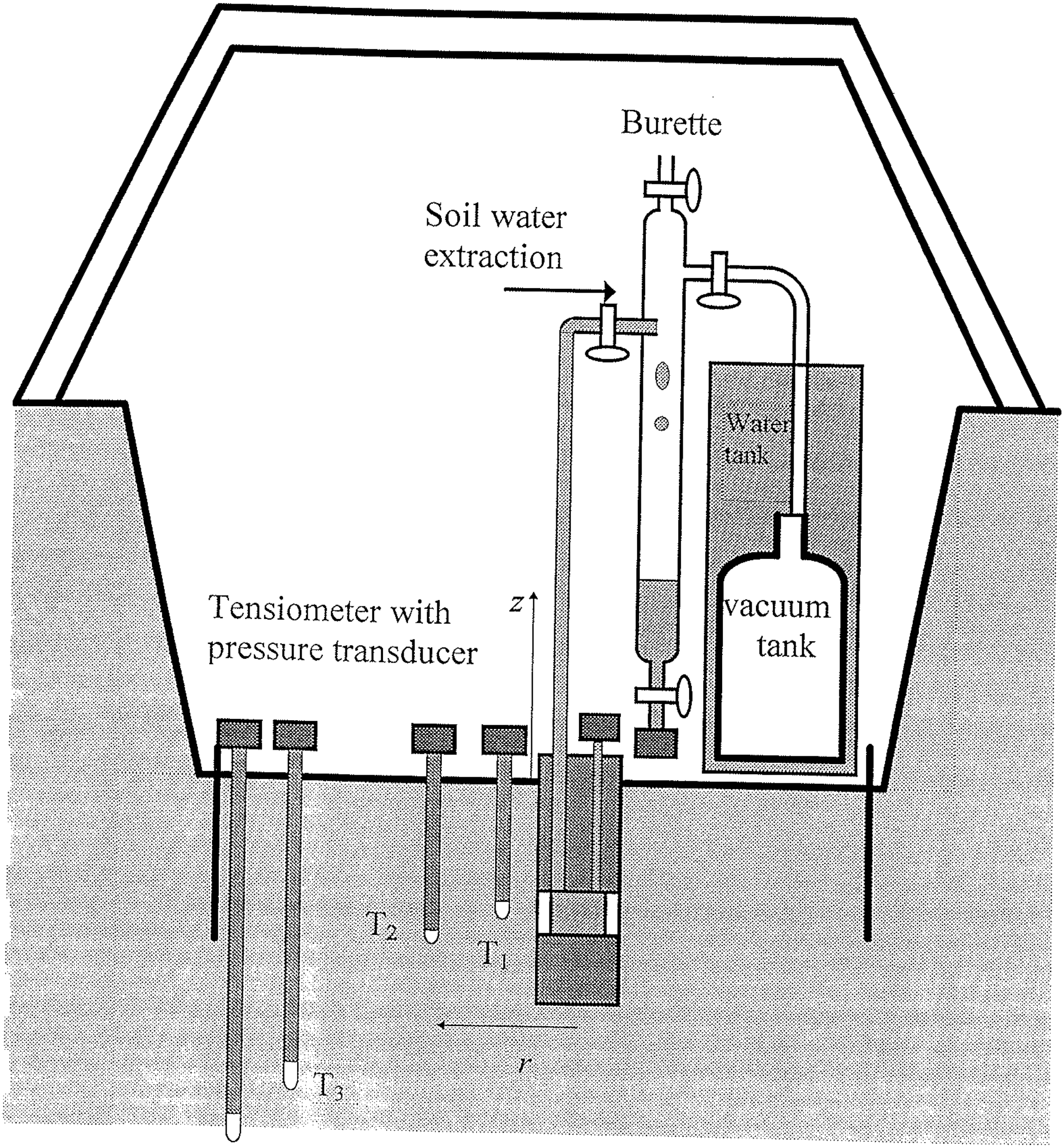

Figure 2. Experimental setup of in situ multi-step extraction experiment

steps were $h_{ex} = -415$ cm for $71.2 < t < 93.0$ h, and $h_{ex} = -685$ cm for $93.0 < t < 120$ h. From core samples at the 60 cm soil depth, measured saturated volumetric water content was 0.56 $cm^3\ cm^{-3}$ and K_s varied between 2.12 and 2.94 cm h^{-1}. Time zero for the computer simulations was at the conclusion of the infiltration test. During the extraction experiment, soil samples representing the 10 cm soil depth were collected and volumetric water content was determined from oven-drying. These volumetric water content data were matched with soil water potential values of the T_1 tensiometers, resulting in the following $\theta - h$ (cm) points: (0.39, -94), (0.36, -133), and (0.35, -149). Also these three independently measured soil water retention points were included in the OF (9). In addition to the tensiometers used to measure response to soil water extraction, additional tensiometers were installed at depths of –8 and –20 cm, at distances of more than 20 cm away from the ceramic extraction device. These matric potential measurements were not influenced by water extraction, and together with the 40 and 55 cm deep tensiometers characterized the draining of the soil profile by gravity forces. Therefore, these matric potential measurements in combination with water content measurements using a neutron probe at depths of 25, 40, 55 and 70 cm were used to obtain additional independent estimates of in situ $\theta(h)$ and $K(\theta)$ data using the instantaneous profile method.

RESULTS AND DISCUSSION

Laboratory experiment (Combined probe)

Interaction between the solution sampler and tensiometer of the combined probe can occur in two ways. First, the vacuum applied to extract soil solution may reduce the soil water pressure measured by the tensiometer compartment. This type of interaction is minimized by increasing the distance between the two compartments and by the measurement of soil water pressure before soil solution is extracted. Second, soil solution concentration may change because of diffusion of solutes between the soil and tensiometer compartment, or by exchange of water between the soil and tensiometer compartment through the porous ceramic. Concerns with regard to potential interactions between the tensiometer and solution extraction compartments led to an improved design, which has been successfully used for field monitoring. The field-tested tension-solution probe is identical to the presented sampler, except that the length of the spacer separating the two compartments was increased. As a result, the distance between the two compartments is larger and interactions between the solution sampler and tensiometer are minimized. The recommended separation distance of a combined field probe is approximately 10 cm. Although this distance is somewhat arbitrary, theoretical considerations indicate that the required minimum separation length is about that distance. The influence of the applied vacuum of the solution sampler on the soil water pressure will depend on many factors, such as flow regime (steady or transient), extraction vacuum, soil hydraulic conductivity, and size and conductance of the extraction device.

Diffusion of soil solution chloride into the tensiometer compartments of the combined samplers, which were filled with deionized water, resulted in an increase of chloride concentration in the tensiometer compartments. Also this type of interaction is minimized by increasing the separation distance between the two ceramic compartments.

The data showed an increasing Cl-concentration as the soil water pressure decreases (with increasing time) as caused by the larger suction increments to the tension table. Since the size of the water-filled pores decreases as the soil water pressure decreases, our data indicate that the pore water concentration is higher in the smaller solution-filled pores. The increase in Cl-concentration with a decrease in solution-filled pore size might be caused by anion exclusion, as the relative exclusion volume increases with decreasing soil water content. This could also explain the larger concentration increase in finer-textured soils, since anion exclusion would be most apparent for higher clay content soils, as these would potentially have a larger anion exclusion volume.

Field experiment (in situ estimation of soil hydraulic functions)

The soil water extractor was the same as used in the laboratory experiments with a measured K_{cer} value of 0.0008334 cm h^{-1}. However parameter optimizations using this value were not very successful with relatively large differences between observed and measured extraction volume and soil water potential values. Hence, in addition to the soil hydraulic parameters, also the conductivity of the ceramic cup, K_{cer}, was optimized. The optimized parameter values are listed in Table 1 (fixed K_{cer}). Using a K_{cer} of 0.000282 the fit for the field experiment was extremely good, reducing the OF-value with on order of magnitude. From the information included into the objective function, i.e., the cumulative extracted volume and tensiometer readings it is not possible to estimate simultaneously both θ_r and θ_s, since these two parameters are fully correlated. It is possible either to fix one of these two parameters and to optimize the other, or to optimize the water content interval $\Delta\theta = \theta_s - \theta_r$. Both approaches should result in similar results. We fixed θ_s at the independently measured value (0.560) and estimated θ_r. The results of Table 1 also show the large uncertainty of the saturated hydraulic conductivity K_s for which the value of *NSD* is always larger than 70%.

In addition to cumulative extraction volume and soil matric potential values at three locations, we also included the three independently measured θ(h) points during the extraction experiment in the objective function. Table 1 also lists the parameter estimates of this final case (Fitted ceramic + θ(h) data). A comparison between measured and calculated cumulative extraction volumes and tensiometer readings (not shown here) shows that the fit of experimental with fitted cumulative extraction volumes and matric potential values for T_2 and T_3, is similar as for the previous cases.

Table 6. Parameter estimation results for field experiment.

	Fixed K_{cer}		Fitted K_{cer}		Fitted K_{cer} + θ *(h) data*	
	Value	*NSD*[1] (%)	Value	*NSD*[1] (%)	Value	*NSD*[1] (%)
α (cm^{-1})	0.0347	20.6	0.0231	23.4	0.0220	30.0
n	1.730	3.01	1.688	2.2	2.313	6.0
θ_s	0.560	-	0.560	-	0.552	11.9
θ_r	0.441	2.76	0.441	3.34	0.301	1.3
K_s (cm h^{-1})	8.530	72.7	3.28	74.4	9.725	119.8
K_{cer} (cm h^{-1})	0.00191	-	0.000282	3.5	0.00026	3.9
OF(b)	0.1105		0.0109		0.0787	

[1] *NSD*: Normalized standard deviation, $100\sigma/b_j$ (%), estimated from parameter variance.

Figure 3 presents the optimized soil water retention and hydraulic conductivity functions for the fitted K_{cer} case with and without the independently determined θ(h) data, as well as the soil hydraulic data estimated independently by the instantaneous profile

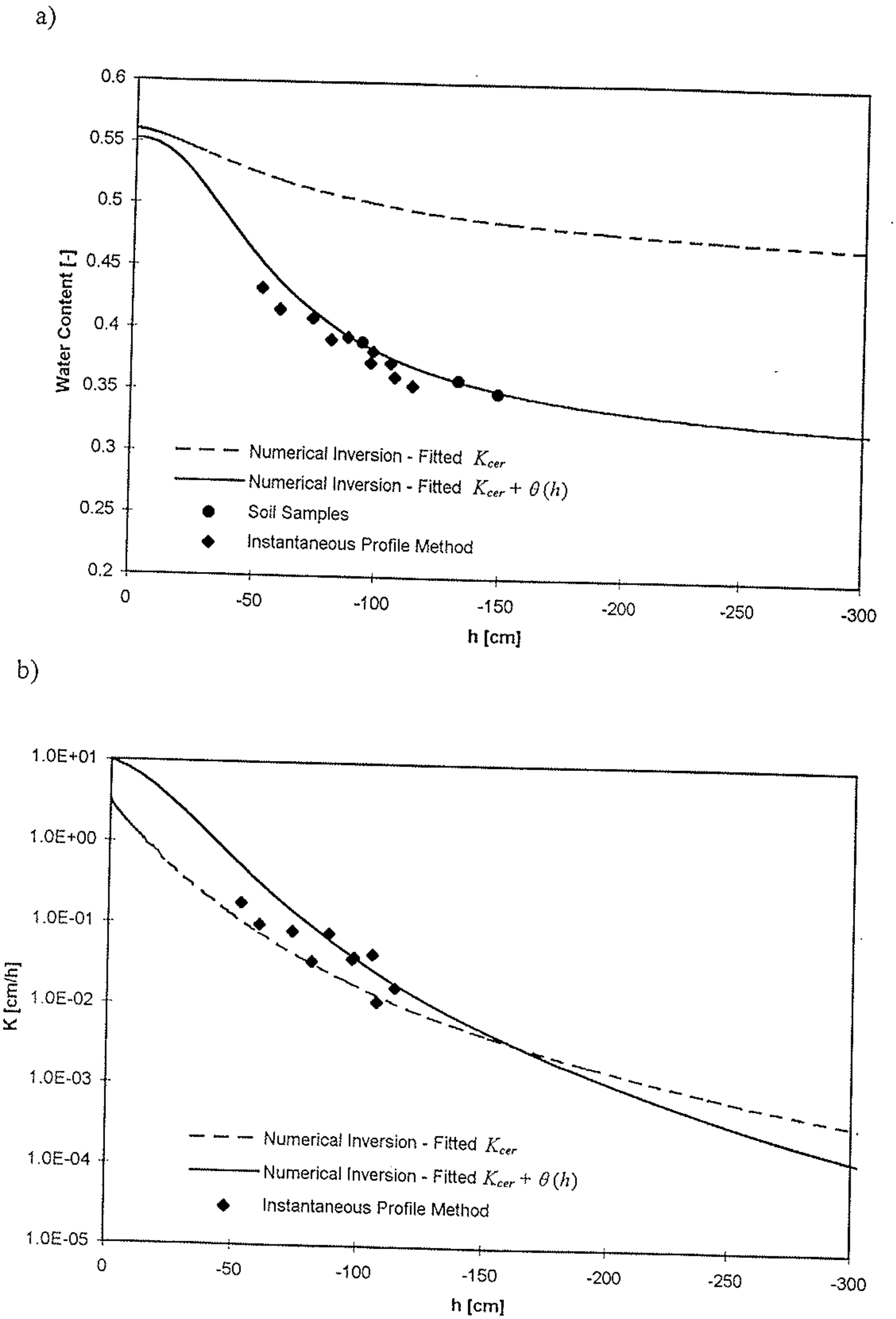

Figure 3. Estimated soil water retention (a) and hydraulic conductivity (b) functions for the two optimization options of Table 1 for Yolo clay loam, compared with independently determined retention and unsaturated hydraulic conductivity data (diamonds).

method (diamond symbols). Figure 3a also includes the 3 $\theta(h)$ points (solid circles). Both optimized soil water retention and unsaturated hydraulic conductivity functions closely approximate the independently estimated retention and unsaturated hydraulic conductivity data in the range between -150 and -50 cm. However, the optimized parameters and hydraulic functions are only valid for the soil matric potential range from near saturation to about -250 cm, i.e., the range over which the extraction experiment was carried out. Continued soil water extraction after 5 days would have generated soil matric potential data smaller than measured in the described field experiment.

PRINCIPAL FINDINGS AND CONCLUSIONS

An instrument capable of measuring soil water and collecting soil solution simultaneously was developed and tested in laboratory conditions for homogeneous soils. However, to minimize interactions between the two compartments of the combined probe, it is recommended to increase the distance between the compartments as compared with the presented design. Combined tension-solution sampling probes using the larger separation distance between compartments have been successfully used for in situ soil solution extraction and soil water pressure monitoring. Laboratory experiments indicated that data obtained with the combined tension-solution sampling probe were close to the conventional tensiometer and soil solution samplers. Differences in soil water pressure between the single and combined probe were attributed to differences in sampling volume of two types of probes. The increase in pore water concentration with a decrease in soil water pressure could be attributed to anion exclusion. In either application, correct characterization of the soil water status of soils is controlled by the size of the sampling volume relative to the representative elementary volume of the soil.

We introduced a new method for effectively estimating soil hydraulic parameters in-situ from a transient flow experiment. The experiment involves extraction of soil solution using successively increasing vacuum steps from an initially near-saturated soil. The extracted volume and measured soil matric potential values at several locations near the soil water extraction device are measured. The soil hydraulic parameters are obtained by minimization of the objective function, which includes the deviations between simulated and experimental data.

Parameter optimization was highly successful if the saturated hydraulic conductivity of the extractor (K_{cer}) was optimized simultaneously with the soil hydraulic parameters, rather than assuming it's independently measured value. We hypothesize that K_{cer} is changing during the extraction experiment because of reduction of hydraulic contact between the ceramic ring and the surrounding soil as the soil desaturates. Optimized soil water retention and unsaturated hydraulic conductivity data corresponded well with independent estimates obtained from the instantaneous profile method in the same experimental plot. However, care should be taken in extrapolating the optimized hydraulic functions beyond the water content range for which the experimental data were obtained.

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