

## Multi-functional heat pulse probe measurements of coupled vadose zone flow and transport

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### Abstract

Simultaneous measurement of coupled water, heat, and solute transport in unsaturated porous media is made possible with the multi-functional heat pulse probe (MFHPP). The probe combines a heat pulse technique for estimating soil heat properties, water flux, and water content with a Wenner array measurement of bulk soil electrical conductivity. To evaluate the MFHPP, we conducted controlled steady-state flow experiments in a sand column for a wide range of water saturations, flow velocities, and solute concentrations. Flow and transport processes were monitored continuously using the MFHPP. Experimental data were analyzed by inverse modeling of simultaneous water, heat, and solute transport using an adapted HYDRUS-2D model. Various optimization scenarios yielded simultaneous estimation of thermal, solute, and hydraulic parameters and variables, including thermal conductivity, volumetric water content, water flux, and thermal and solute dispersivities. We conclude that the MFHPP holds great promise as an excellent instrument for the continuous monitoring and characterization of the vadose zone.

*Key words:* Heat pulse probe; unsaturated flow; heat transport; solute transport; vadose zone properties; water content; water flux; dispersion.

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### 1 Introduction

Multi-functional measurements of vadose zone processes have received increased attention over the past few years. New sensors are being developed, by which several already well-known measurement techniques are combined into a single device. The overall motivation for the development of these multi-functional techniques is to achieve an improved characterization of flow and transport processes. Several benefits are achieved by combining measurements. First, by measuring several parameters at the same time and place, the coupling of related transport properties are determined in concert, thereby allowing examination of the nature of their interdependency, such as for the coupled transport of water and solute, and water and heat. Second, by using the same instrument for various measurements within approximately the same measurement volume at about the same time, the need to interpolate different measurement types in space and time is largely eliminated. Thirdly, simultaneous analysis of flow and transport using combined soil measurements of water content, temperature, and solute concentration, decreases parameter uncertainty. Thus, using multi-functional measurement techniques allows determination of inter-dependent soil properties and processes, providing an improved understanding of coupled flow and transport.

The presented multi-functional heat pulse probe (MFHPP) originates from the dual-probe heat pulse (DPHP) method developed by Campbell et al. (1991). By inducing a short heat pulse from one sensor needle and measuring the temperature response at a second sensor, the soil thermal properties (i.e., heat capacity,  $C_{bulk}$ ; thermal conductivity,  $\lambda_0$ ; and thermal diffusivity,  $\kappa$ ) and the water content,  $\theta$ , were estimated. This method has been tested in both laboratory settings (Basinger et al., (2003; Bristow, 1998) and in field soils (Heitman et al., 2003). Over the past few years, the DPHP probe has been refined and

was developed into various multi-sensor probes that are capable of simultaneous measuring a suite of soil properties. The potential of measuring bulk soil electrical conductivity,  $EC_{bulk}$ , using a modified heat pulse probe was shown by Bristow et al. (2001) by including two extra sensor needles in the DPHP probe to create a so-called four-electrode Wenner array. Since  $EC_{bulk}$  measurements are dependent on both solute concentrations and water contents,  $EC_{bulk}$  is an integral variable characterizing both water flow and solute transport that can be beneficially used to simultaneously estimate soil hydraulic and solute transport parameters.

By inclusion of an extra temperature sensor to measure both the temperature responses at the upstream and downstream end of the heater sensor, Ren et al. (2000) demonstrated the added benefit of water flux estimation. The multi-functional heat pulse probe (MFHPP) of the current study combines this type of heat sensor with a 4-needle Wenner array. As demonstrated by Mori et al. (2003, 2005), the MFHPP allow estimation of the soil thermal properties (i.e., thermal conductivity, and thermal diffusivity), simultaneously with the soil water properties (water content and water flux). Furthermore, the MFHPP estimates  $EC_{bulk}$  from Wenner array measurements, from which the soil's solute concentration and water content can be determined.

In this study, the MFHPP technique was applied in flow and transport column experiments for the simultaneous and coupled measurement of water, heat, and solute transport variables and properties. Controlled steady-state flow experiments through variably-saturated sand were conducted for a range of water flux, water saturation, and solute concentration values. Heat pulse and  $EC_{bulk}$  measurements were analyzed with inverse modeling using a modified version of the HYDRUS-2D code (Šimůnek et al., 1999). The main objective of the presented study was to evaluate the MFHPP as a means to fully characterize coupled soil water flow, heat, and solute transport properties and processes.

## 2 Materials and Methods

Soil thermal and hydraulic properties were evaluated from analysis of temperature responses of the thermistors of the MFHPP, solving for heat transport by both conduction and convection. Solution of solute transport is needed for interpretation of bulk soil electrical conductivity ( $EC_{bulk}$ ) measurements. The presented analysis will solve the coupled heat, water, and solute transport equations using HYDRUS-2D (Simunek et al., 1999; Hopmans et al., 2002):

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left[ \kappa_{xx} \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial z} \left[ \kappa_{zz} \frac{\partial T}{\partial z} \right] - \left[ V_h \frac{\partial T}{\partial z} \right] \quad (1)$$

where  $T$  is temperature (K),  $t$  is time (s),  $z$  is vertical position (m),  $\kappa_{zz}$  and  $\kappa_{xx}$  denote the effective thermal diffusivities ( $\text{m}^2 \text{s}^{-1}$ ) in the  $z$  and  $x$  directions, and  $V_h$  denotes the convective heat pulse velocity ( $\text{m s}^{-1}$ ):

$$V_h = \frac{C_w q_{w,z}}{C_{bulk}} = \frac{\theta C_w v_w}{C_{bulk}} \quad (2)$$

where  $C_w$  is the heat capacity of water ( $\text{J m}^{-3} \text{K}^{-1}$ ),  $C_{bulk}$  is the volumetric heat capacity of bulk soil ( $\text{J m}^{-3} \text{K}^{-1}$ ), and  $v_w = q_{w,z}/\theta$  is the average pore water velocity ( $\text{m s}^{-1}$ ). Equation 2 describes heat flow by moving liquid phase, relative to the stationary bulk porous medium. Steady-state variably saturated water flow in the  $z$ -direction is described by the Darcy flux,  $q_{w,z}$  ( $\text{m s}^{-1}$ ):

$$q_{w,z} = -K(\theta) \left( \frac{\partial h_m}{\partial z} + 1 \right) \quad (3)$$

where  $K(h_m)$  is the hydraulic conductivity function ( $\text{m s}^{-1}$ ) and  $h_m$  is the soil water matric head (m).

Assuming single domain transport for a conservative tracer with steady-state water flow, one-dimensional solute transport of our experiments is described by the conventional advection-dispersion equation:

$$\theta \frac{\partial C}{\partial t} = \frac{\partial}{\partial z} \left( \theta D \frac{\partial C}{\partial z} \right) - v_w \frac{\partial \theta C}{\partial z} \quad (4)$$

where  $C$  is the solute concentration ( $\text{kg m}^{-3}$ ),  $D$  is the effective solute dispersion coefficient ( $\text{m}^2 \text{s}^{-1}$ ). Assuming that molecular diffusion is negligible, the hydrodynamic dispersion coefficient reduces to:

$$D = \alpha_L(\theta)v_w \quad (5)$$

where  $\alpha_L$  is the longitudinal solute dispersivity (m). The four horizontal sensors of the MFHPP were used as a four-electrode Wenner array sensor for bulk soil electrical conductivity ( $EC_{bulk}$ ) measurements (Mori et al., 2003). The  $EC_{bulk}$  value depends on the solution electrical conductivity,  $EC_w$  ( $\text{mS cm}^{-1}$ ), the soil surface conductivity,  $EC_s$  ( $\text{mS cm}^{-1}$ ), soil water content,  $\theta$ , soil bulk density,  $\rho$ , temperature,  $T$ , and sensor geometry. Assuming the Rhoades et al. (1976) relationship to be valid and neglecting the soil surface conductance of the sandy soil,  $EC_{bulk}$  is given by:

$$EC_{bulk} = c_1 EC_w \theta^2 + c_2 EC_w \theta \quad (6)$$

where  $c_1$  and  $c_2$  are empirical parameters.

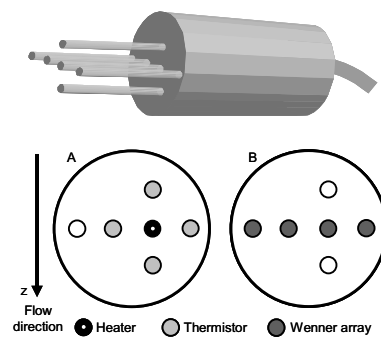


Figure 1. Schematic of the MFHPP design, with heat pulse measurement using the central heater sensor and the four surrounding thermistors (A) and EC measurements using the horizontal four-needle Wenner array (B).

The heat flow equation (Eq. 1) above was solved simultaneously with the steady-state flow and the conventional advection-dispersion equation, to solve for solute concentration and flux. Flow column experiments were performed to examine steady-state flow and transport for a range of water saturation, water velocity, and solute concentration values. The MFHPP by Mori et al. (2003, 2005) was used to monitor coupled heat, water, and solute transport. The MFHPP is constructed from six sensors (26 mm long and 1.27-mm O.D. stainless steel needles), which are incorporated into a 27-mm radius probe with approximately 6 mm distance between the sensors (Fig. 1). The six sensors include a single central heater sensor, four thermistor sensors located around the heater, and the four-needle Wenner array. Heat pulse experiments are conducted by generating an 8-second heat pulse at the central heater sensor, corresponding to a heat flux of about  $60 \text{ W m}^{-1}$ , after which the temperature responses at the surrounding thermistor sensors are measured. Steady-state water flow experiments were conducted in a 7.94-cm inner diameter and 30 cm long Plexiglas column packed with 28 cm of Tottori Dune sand (Fig. 2). Flow through the sand column was controlled through application of a range of steady-state water flux values,  $q_{w,z}$ , between 0 and  $17.84 \text{ m d}^{-1}$ , with corresponding variable suction at the bottom boundary. Assuming spatial uniformity, these steady state water fluxes were achieved by an artificial 12-needle rainmaking device. The soil water matrix potential was measured with miniature tensiometers with a 1 cm long and 0.635-cm O.D. ceramic cup. Tracer solutions were mixed prior to the experiments by adding  $\text{CaCl}_2$  to distilled water, achieving a range of concentrations of 0.01, 0.03, 0.06, 0.08, and  $0.1 \text{ mol L}^{-1}$ .

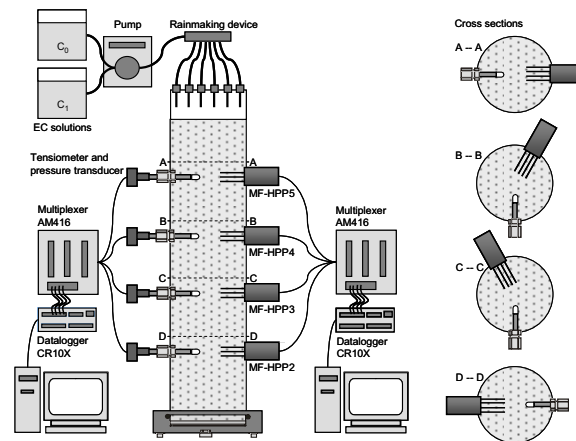


Figure 2. Schematic of the experimental flow column. The relative positions of the MFHPP's and tensiometers are presented in the cross-sections (right): A-A at 4 cm depth, B-B at 10 cm depth, C-C at 16 cm depth, and D-D at 22 cm depth.

As presented in Mortensen et al. (2005), inverse modeling techniques were applied for analysis of the experimental data, allowing simultaneous estimation of soil thermal properties (heat conductivity, heat dispersivity, and heat diffusivity) and solute properties (solute concentration and solute dispersion) that are coupled through the soil water properties of water content and water flux. Most importantly, inverse modeling allows for the simultaneous estimation of coupled flow and transport parameters. Furthermore, both the number and the type of measurements to be included in the optimization can be varied. We used the HYDRUS-2D finite element code by Šimůnek et al. (1999) for analysis of the MFHPP experiments. The code solves simultaneously water flow with heat and solute transport in two spatial dimensions ( $x$  and  $z$ ). It considers heat transport by conduction, convection, and dispersion, and solute transport by Fickian-based advection-dispersion. HYDRUS-2D uses the Levenberg-Marquardt (LM) algorithm for parameter optimization by inverse modeling. The experiments were simulated for a 3.97 cm (horizontal) by 28 cm (vertical) transport domain, corresponding to the radius and the height of the sand column. For the heat pulse experiments, the objective function  $\Phi$  to be minimized during the parameter estimation was defined as follows

$$\Phi(\mathbf{p}_{\text{HP}}) = W_1 \sum_{i=1}^{N_1} [T^*(\mathbf{x}, t_i) - T(\mathbf{x}, t_i, \mathbf{p}_{\text{HP}})]^2 \quad (6)$$

where the right hand side represents the residuals between measured temperatures,  $T^*$ , and corresponding predicted temperatures,  $T$ . The vector  $\mathbf{x}$  denotes the spatial coordinate of each measurement  $i$ ,  $N_1$  the total number of temperature measurements,  $W_1$  is the weight associated with a particular measurement data point, and the vector  $\mathbf{p}_{\text{HP}}$  contains the optimized parameters.

### 3 Results and Discussion

Measured temperature differences of all four thermistors for each MFHPP device were used to estimate both soil thermal and hydraulic parameters. As an example, we present a comparison of measured with optimized temperature signals for unsaturated experiments at zero-flow and at steady state flow of  $q_{w,z} = 6.25 \text{ m d}^{-1}$  in Fig. 3. In the absence of water flow, heat is transported by conduction only, resulting in symmetrical spreading of the heat pulse around the heater needle to all 4 surrounding thermistors equally, with slight variations caused by variable sensor spacing and soil heterogeneities. In contrast, asymmetrical temperature responses occur for the steady-state flow water experiments with heat convection, resulting in temperature differences between the upstream, downstream, and transverse thermistor locations (Hopmans et al., 2002). However, in either case, the temperature response will increase with decreasing soil water content. EC measurements were analyzed to estimate solute dispersivity and water flux, with and without simultaneous temperature response measurements.

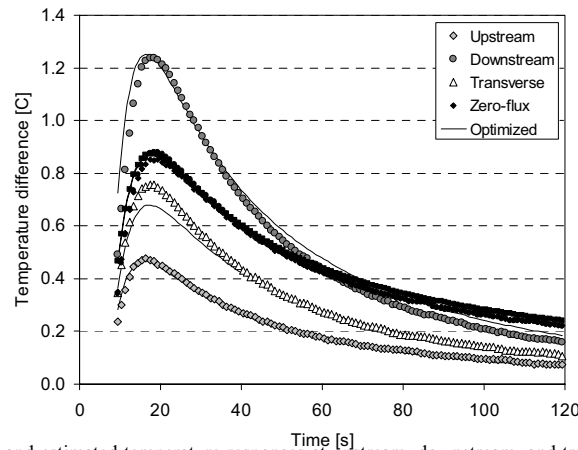


Fig. 3. Example of measured and estimated temperature responses at upstream, downstream, and transverse thermistor sensors for unsaturated experiments with no flow ( $\theta = 0.147$ ;  $q_{w,z} = 0 \text{ m d}^{-1}$ ) and steady-state flow ( $\theta = 0.213$ ;  $q_{w,z} = 6.25 \text{ m d}^{-1}$ ).

3.1 Thermal and hydraulic properties from single MFHPP measurements

The single probe optimizations of both unsaturated zero-flow and steady state experiments included estimations of the volumetric water content,  $\theta$ . These estimated water content values are compared with the corresponding simulated water content values from hydraulic parameters in Fig. 4A, with a RMSE of  $0.019 \text{ m}^3 \text{ m}^{-3}$ . In our simulations with HYDRUS-2D, temperature data for all four thermistors were included to estimate average water content. Yet, significant differences in water contents with vertical position might occur, because of the large sensitivity of the sand soil moisture to the matric head. Simultaneously with soil water content, the soil thermal conductivity,  $\lambda$  was estimated from both saturated and unsaturated experiments for both zero-flux and a series of steady-state flow conditions. Estimated thermal conductivities for all experiments combined are presented in Fig. 4B as a function of the soil water content, as estimated from the MFHPP measurements. Our data compared remarkably well with the independent sandy soil data of Hopmans and Dane (1986), as was also found from previous work by Mori et al. (2003, 2005), who used the MFHPP technique in combination with analytical solutions.

In addition to water content and thermal properties, the single probe optimizations also yielded estimated water flux densities. Estimated water fluxes are compared with the true fluxes, as computed from volumetric drainage flow rates in Fig. 4C. More accurate flux estimates were generally obtained for the unsaturated flow experiments (RMSE of  $0.49 \text{ m d}^{-1}$ ) as compared to the saturated experiments (RMSE of  $1.94 \text{ m d}^{-1}$ ), with the mostly higher flow rates. For the saturated flow experiments, water fluxes were generally underestimated, with relative errors between 10 and 20%. For the unsaturated steady state flow experiments, the MFHPP optimizations generally underestimated the flow at high water fluxes as well. Various other studies also concluded that HPP measurements underestimated water flux at high flow rates (Hopmans et al., 2002; Ren et al., 2000). Mori et al. (2003) point out the difficulty in estimating water fluxes if values are smaller than  $0.1 \text{ m d}^{-1}$ . It was suggested that the limitation of the MFHPP in the low water flux range is controlled by the temperature resolution of the thermistors ( $0.01^\circ \text{C}$ ).

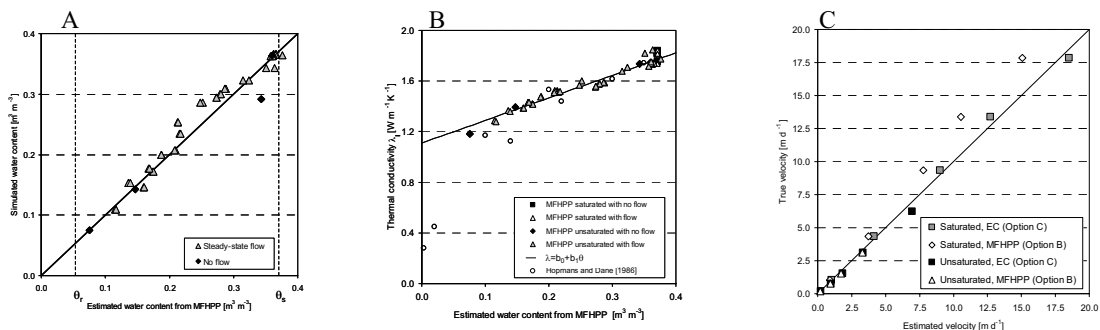


Fig. 4. Soil water content (A), soil thermal conductivity (B) and soil water flux estimates (C) from MFHPP measurements.

### 3.2. Tracer experiments

For the tracer experiments, the objective function consists of  $EC_{bulk}$  values, as measured by the four-electrode Wenner array of the four MFHPP's for each steady state flow experiment. Since the  $EC_{bulk}$  contains information on both solute concentration and volumetric water content, breakthrough measurements were used to simultaneously estimate both soil hydraulic and solute transport parameters. The dependency of water content on  $EC_{bulk}$  resulted in distinctly different breakthrough curves for both the saturated and unsaturated (Fig. 5) flow experiments, with  $EC_{bulk}$  differences at equal concentrations between probes attributed to individual calibration equations. When comparing the results, we also notice the slightly larger noise in concentration values for the unsaturated experiments, even though the average velocity was much larger for the saturated experiments. The unsaturated breakthrough curves showed significant tailing, which has been observed in general for unsaturated breakthrough curves. The optimized water flux values are compared in Fig. 4C with the true water fluxes. RMSE values were 0.458

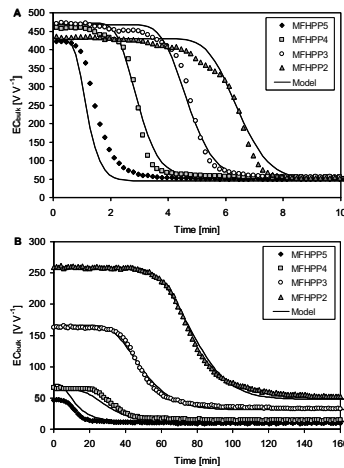


Figure 5. Example of measured and estimated  $EC_{bulk}$  breakthrough curves for (A) saturated flow at  $q_{w,z}=17.84 \text{ m d}^{-1}$  and (B) unsaturated flow at  $q_{w,z} = 0.78 \text{ m d}^{-1}$ . Measured  $EC_{bulk}$  is both a function of the probe and the water content, which is described by individual calibration equations.

and  $0.357 \text{ m d}^{-1}$  for the saturated and unsaturated experiments, respectively. Generally, the tracer optimizations gave better flux estimates for the saturated experiments, especially for the high flux experiments. This is not surprising as solute breakthrough is largely controlled by convection, especially for the relatively high water fluxes of this experiment. For the unsaturated experiments, very similar optimization results were found for the tracer experiments and the heat pulse experiments.

## 4 Conclusions

The new MFHPP technique combined with inverse modeling allowed for simultaneous estimation of coupled thermal, hydraulic, and solute properties. Single probe inverse optimization allowed simultaneous estimation of thermal characteristics, such as thermal conductivity and heat dispersion, soil hydraulic properties, water flux density and volumetric water content. Estimated parameters were generally in good agreement with independently-measured values. The main advantage of multiple probe optimizations is that the water content dependency of thermal and hydraulic relationships could be determined simultaneously from the coupled column experiments, provided that a wide range in experimental water content values can be achieved. The Wenner array of the MFHPP provided for bulk soil  $EC$  measurements during tracer breakthrough. The combination of MFHPP measurements with inverse numerical analyses is shown to be a promising method for the simultaneous analysis of coupled water, heat, and solute flow processes in variably-saturated porous media.

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