# Development and Optimization of a Multifunctional Sensor for Measuring Soil Thermal Properties, Water Retention Characteristics and Electrical Conductivity

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#### Abstract

Soil water content, matric potential, thermal properties, and electrical conductivity are fundamental and interrelated properties required by a variety of applications in soil science, hydrology, agriculture, and engineering. However, the measurements of the properties are affected by the temporal and spatial variability of soil due to employment of a variety of sensors, which hinders the research and modeling of coupled water, heat and solute transport. In addition, the laborious, costly and time-consuming sensor optimization is always a challenge for traditional sensor development. The objective of this study was to develop a multifunctional sensor integrating heat pulse, time domain reflectometry and porous ceramic matrix and optimize the sensor with COMSOL based numerical simulations. COMSOL simulated ceramic properties (e.g., thermal conductivity, volumetric heat capacity, dielectric permittivity, electrical conductivity) and soil properties (e.g., thermal conductivity and volumetric heat capacity) with different scenarios of sensor dimensions (e.g., the radius and length of the ceramic and extended rod length) were systematically evaluated and verified with experimental data. Our results show that the optimal radius and length of the ceramic are 18 mm and 40 mm, respectively, and the optimal rod length extended out of the ceramic is 50 mm. The optimized results indicate low estimation errors for dielectric permittivity ( $\pm 1\%$ ), electrical conductivity ( $\pm 2\%$ ), and volumetric heat capacity ( $\pm 1\%$ ) of the ceramic as well as thermal conductivity ( $\pm 3\%$ ) and volumetric heat capacity ( $\pm 1\%$ ) of soil. The new multifunctional sensor can provide accurate measurement and modeling of soil hydrothermal properties.

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Development and Optimization of a Multifunctional Sensor
for Measuring Soil Thermal Properties, Water Retention
<b>Characteristics and Electrical Conductivity</b>
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Highlights
• By coupling porous ceramic matrix to heat pulse and time domain
reflectometry, a multifunctional sensor which can simultaneously measure
soil thermal properties, water retention characteristics and electrical
conductivity was developed
• COMSOL simulations were used to optimize sensor dimension and verified
with experimental measurements
• Considering the different combinations of porous ceramic matrix and soil
water content, the measurement errors of soil thermal conductivity (288
treatments) and porous ceramic matrix thermal conductivity (including the

1

- errors caused by radial heat conduction and axial heat conduction, 288
  treatments respectively), dielectric permittivity (3960 treatments) and
  electrical conductivity (5940 treatments) were evaluated
- Porous ceramic matrix radius of 18 mm, ceramic length of 40 mm and
   extended rod length of 50 mm is the optimal sensor design

#### 30 Abstract:

Soil water content, matric potential, thermal properties, and electrical 31 32 conductivity are fundamental and interrelated properties required by a variety of 33 applications in soil science, hydrology, agriculture, and engineering. However, the 34 measurements of the properties are affected by the temporal and spatial variability of 35 soil due to employment of a variety of sensors, which hinders the research and 36 modeling of coupled water, heat and solute transport. In addition, the laborious, costly 37 and time-consuming sensor optimization is always a challenge for traditional sensor 38 development. The objective of this study was to develop a multifunctional sensor 39 integrating heat pulse, time domain reflectometry and porous ceramic matrix and 40 optimize the sensor with COMSOL based numerical simulations. COMSOL simulated 41 ceramic properties (e.g., thermal conductivity, volumetric heat capacity, dielectric 42 permittivity, electrical conductivity) and soil properties (e.g., thermal conductivity and 43 volumetric heat capacity) with different scenarios of sensor dimensions (e.g., the 44 radius and length of the ceramic and extended rod length) were systematically 45 evaluated and verified with experimental data. Our results show that the optimal 46 radius and length of the ceramic are 18 mm and 40 mm, respectively, and the optimal 47 rod length extended out of the ceramic is 50 mm. The optimized results indicate low 48 estimation errors for dielectric permittivity  $(\pm 1\%)$ , electrical conductivity  $(\pm 1\%)$ , 49 thermal conductivity ( $\pm 2\%$ ), and volumetric heat capacity ( $\pm 1\%$ ) of the ceramic as 50 well as thermal conductivity ( $\pm 3\%$ ) and volumetric heat capacity ( $\pm 1\%$ ) of soil. The 51 new multifunctional sensor can provide accurate measurement and modeling of soil 52 hydrothermal properties.

53 Keywords: Thermo-TDR, thermal/heat dissipation, matric potential, heterogeneity,
54 measurement sensitivity, finite element simulation

Abbreviations: AC/DC, alternating current/direct current; DPHP, dual-probe heat
pulse; Ho, homogeneous soil without ceramic; I, rods subjected to inward deflection;
ILS, infinite line source; M, measured data; *MSC*, measurement sensitivity to the

- 58 ceramic; *MSS*, measurement sensitivity to the soil; N, rods subjected to no deflection;
- 59 O, rods subjected to outward deflection;  $RE_a$ , absolute value of relative error; RMSE,
- 60 root means square error; S, simulated data; STP, soil thermal properties; SWRC, soil
- 61 water retention characteristics; TDR, time domain reflectometry; Thermo-TDR, heat
- 62 pulse-time domain reflectometry.

#### 63 **1 Introduction**

64 Soil thermal properties (STP) and soil water retention characteristics (SWRC) 65 determining the soil thermal dynamics, status and momentum of water (e.g., ice, liquid water or vapor), affecting a series of processes such as crop growth and 66 development (Nagai and Makino 2009), soil structure change (Zhang et al. 2017), 67 68 water and energy exchange between land and atmosphere (Brocca et al. 2013), and 69 distribution of solute, gas, water and energy in soil (Mortensen et al. 2006). They are 70 therefore closely related to hydrological, meteorological, agricultural, engineering, 71 ecological environment and geophysical research (Saito et al. 2006). Among them, SWRC represents the relationship between water content ( $\theta$ , cm<sup>3</sup> cm<sup>-3</sup>) and matric 72 potential ( $\psi_m$ , kpa), and STP are important parameters for evaluating surface energy 73 and geothermal resources, which mainly include thermal conductivity ( $\lambda$ , W 74 m<sup>-1</sup> °C<sup>-1</sup>), volumetric heat capacity (C, M J m<sup>-3</sup> °C<sup>-1</sup>), and thermal diffusivity ( $\kappa$ , m<sup>2</sup> 75  $s^{-1}$ ). Accurate, non-destructive, continuous and simultaneous monitoring of these 76 77 properties at both laboratory and field is therefore of great significance, especially 78 with the development of smart agriculture and hydrology (Lekshmi et al. 2014; 79 Bwambale et al. 2022; Datta and Taghvaeian 2023).

80 A variety of techniques for measuring SWRC and STP have been developed. For 81 instance, the dual-probe heat pulse (DPHP) method (He et al. 2018), time domain 82 reflectometry (TDR) method (Robinson et al. 2003; He et al. 2021; He et al. 2023), 83 and ceramics or gypsum based matric potential sensors are currently the most widely 84 used techniques to continuously, rapidly and accurately measure STP,  $\theta$  and electrical conductivity (EC,  $\sigma$ ), and  $\psi_m$ , respectively in both laboratory and field. These methods 85 86 share similarities in measuring principles. For example, DPHP estimate STP based on 87 transport of heat by solving the heat transport equation and TDR measure soil water 88 content based on the dielectric permittivity of water that is much greater than other 89 soil components (e.g., 80 for water vs 5-10 for other components at room 90 temperature). Existing matric potential sensors estimate soil matric potential by 91 indirectly measuring change of soil water content (Noborio et al. 1996; Or and Wraith 92 1999), thermal conductivity or heat capacity (Phene et al. 1971; Reece 1996; Kojima 93 et al. 2017; Kojima et al. 2021), or electrical resistance or conductivity (Xin et al. 94 2007) of a porous ceramic or gypsum matrix in equilibrium with its surrounding soils. 95 However, employment of the abovementioned DPHP, TDR and matric potential 96 sensors is affected by unmatched measurement frequency, sensing volume and 97 installation locations between the sensors due to the highly temporal and spatial 98 variability of the soil. This is among the dominant challenges for coupled water and 99 heat transport.

100 Previous studies have attempted to combine these methods for measuring 101 multiple soil properties with satisfactory performance. For instance, coiled TDR 102 (Noborio et al. 1999; Scanlon et al. 2002; Lungal and Si 2008) or time domain 103 transmissometry (Kojima et al. 2023) was incorporated into ceramics or gypsum to 104 simultaneously measure both water content and matric potential to obtain the SWRC, 105 which describes the change of water content as a function of matric potential. Ren et 106 al. (1999) combined DPHP and time domain reflectometry to develop the thermo-TDR or T-TDR technique for continuous and simultaneous measurement of  $\theta$ ,  $\sigma$ , 107 108 temperature (T), C,  $\lambda$  and  $\kappa$  of the same soil sample. However, thermo-TDR cannot 109 measure  $\psi_m$  that is needed to study soil water movement and the short TDR needs to 110 be calibrated for accurate estimate of  $\theta$  (He et al. 2015; He et al. 2018). Kojima et al. 111 (2021) incorporated part of DPHP sensor into a ceramic block to simultaneously 112 estimate  $\theta$ , C, and  $\lambda$  (by DPHP) as well as  $\psi_m$  (by ceramics) of the same soil sample. 113 However, it indirectly estimates soil water content with additional known information 114 (e.g., bulk density,  $\rho_b$ ) and would introduce extra uncertainties in measurement 115 without calibrations and limits its application in the field to continuously monitor  $\theta$ 116 (Ren et al. 2005). Moreover, a soil multifunctional sensor coupling TDR can be used to measure EC (Dalton et al. 1984; Kargas and Soulis 2019; He et al. 2021). Currently 117

there is an urgent need for a multifunctional sensor that enables the fully couple of
DPHP, TDR and porous ceramic matrix for simultaneous measurement of STP and
SWRC.

121 A good design is imperative to the high accuracy of the multifunctional sensor. 122 According to the infinite line heat source (ILS) model, the heater size of DPHP is 123 usually simplified, that is, the heat source of finite length is considered as the heat 124 source of infinite length, and the cylindrical heat source is considered as the linear 125 heat source (Campbell et al. 1991; Bristow et al. 1994). The rod of the DPHP should 126 be slender to conform to the ILS model. However, the design results in a variable rod 127 spacing (r, mm), which increases the measurement error of C (Noborio et al. 1996). A 128 small r allows easier identification of the maximum temperature rise and the time corresponding to the maximum temperature rise at a lower heat strength (q', W m<sup>-1</sup>), 129 effectively avoiding convective heat transfer around the heater. However, a small r130 131 means a higher relative error in determining r and less representative measurements, because of the small sampling volume (Ren et al. 1999). Therefore, the DPHP was 132 designed with a rod length (L) of 28 mm, a rod diameter (d) of 0.8 mm, and an r of 6 133 134 mm (Bristow et al. 1994). To reduce the TDR signal attenuation (which varies with 135 soil texture,  $\theta$ , and  $\sigma$ ) and accurately estimate the travel time, the maximum and 136 minimum rod lengths of the TDR rod can be estimated as (Dalton and Van Genuchten 1986; Ren et al. 1999): 137

138 
$$L_{max} = \frac{\ln\left(\frac{V_T}{V_R}\right) \cdot \sqrt{\varepsilon}}{12\pi\sigma}$$
(1)

139 
$$L_{min} = \frac{t_e v_0}{2\sqrt{\varepsilon}}$$
(2)

140 where  $L_{max}$  and  $L_{min}$  are the maximum and minimum rod lengths (m), respectively,  $V_T$ 141 and  $V_R$  are excitation voltage and reflected voltage (V), respectively,  $\varepsilon$  is dielectric 142 permittivity,  $\sigma$  is electrical conductivity (dS m<sup>-1</sup>),  $t_e$  is the travel time of 143 electromagnetic wave (s), and  $v_0$  is the velocity of light in a vacuum (3 × 10<sup>8</sup> m s<sup>-1</sup>). To avoid the skin effect and excessive soil disturbance, the ratio of rod spacing to rod diameter (r/d) should be as large as possible but less than 10 (Knight 1992). Considering the accuracy of soil thermal properties and water content measurement, the thermo-TDR developed by Ren et al. (1999) was designed with a *L* of 40 mm, *d* of 1.3 mm, and *r* of 6 mm.

149 In addition, traditional sensor optimization requires numerous designs/types 150 (e.g., sensor dimension: rod length and size, rod spacing, material, and heat strategies) 151 for comparison and screening the best-performing sensor design (Or and Wraith 1999; 152 Liu et al. 2008; Kamai et al. 2015; Menne et al. 2022). This approach is effective but 153 costly, time consuming and laborious, the best optimized design may not be properly 154 selected and the sampling volume and interferences among methods may still remain 155 unknown. Therefore, there is a need to introduce numerical simulations to facilitate probe design in order to comprehensively evaluate numerous factors and their 156 157 combinations affecting the sensor, and avoid the effects of uncontrollable sources of 158 error in applications (Zhao et al. 2023). A few previous studies have analyzed various 159 factors affecting the accuracy of TDR or DPHP based on numerical simulation 160 software such as GeoStudio (Zhan et al. 2015), HYDRUS (Saito et al. 2007), and 161 COMSOL (Rakesh et al. 2021; Meng et al. 2023). This approach has been approved 162 effectively and cost effective and led to improvements in sensor design and 163 construction under different measurement conditions, which in turn improved the 164 measurement range, accuracy and precision of newly designed sensors. Numerical 165 simulations have the potential to optimize multifunctional sensors combing the DPHP, 166 TDR and ceramics.

167 Therefore, the objective of this study was to design a soil multifunctional sensor 168 and optimize it using numerical simulation. DPHP, TDR and matric potential sensor 169 were coupled to allow the simultaneous and continuous measurement of SWRC and 170 STP of the same soil, that is, to obtain unified soil hydrothermal data in the same time 171 and space. COMSOL that supports multi-physical field simulations was used to quantitatively analyze the measurement error and to optimize sensor design in terms
of soil-ceramic equilibrium as well as heat (for heat pulse measurements) and
electromagnetic transfer (for TDR measurements).

175 2 Materials and methods

#### 176 **2.1 Porotype sensor development**

177 We developed a soil multifunctional sensor by coupling a porous ceramic matrix to extended thermo-TDR rods (Figure 1). The ceramic was prepared by a sintering 178 179 technology, with raw materials of diatomite, kaolin, dextrin, activated carbon powder 180 and silica sol at a mass ratio of 8: 3: 2: 7: 9. The raw materials were mixed, filled into 181 a specific mold, and pressed at a pressure of 12 Mpa for 3 min. It was sintered in a 182 muffle furnace at 1200 °C for 15 h after drying at room temperature for 24 h. The 183 activated carbon powder was composed of equal weights of five different particle 184 sizes (< 75 µm, 75-250 µm, 125-250 µm, 250-400 µm, and 400-1000 µm) of 185 powder. The activated carbon power was used as a pore-forming agent, which 186 sublimated during sintering, forming numerous pores of different sizes. A ceramic 187 with wide pore size distribution can prevent hydraulic decoupling due to a mismatch 188 between the pore size distribution of the sensor and that of the soil, thus providing 189 maximum sensitivity in the range of matric potential studied (Phene et al. 1971; 190 Malazian et al. 2011; Menne et al. 2022). The thermo-TDR in this study was a 191 traditional three-rod sensor, with rod spacing r of 6 mm and rod diameter d of 1.3 192 mm. The heating wires were placed in the middle rod as a linear heat source. Two 193 thermocouples were placed in each rod to sense the temperature rise of the ceramic 194 and soil. High-thermal-conductivity epoxy glue was then drawn into hollow place 195 next to heating wires and thermocouples in the rods to construct a water-resistant, 196 electrically-insulated rod. The joints of the electrical leads and the heating wires or the 197 thermocouples were soldered. For the TDR part of the sensor, the central rod and two 198 external rods were connected to the positive central lead and metal shield of the

coaxial cable, respectively. The joints of the rods and the electrical leads were thenencased in epoxy as the sensor handle.



201

202 Figure 1. Front view (a) and cross section view (b) of the soil multifunctional sensor.

203 The rod base of the sensor was incorporated into a ceramic (Figure 1). The 204 extended rods were in contact with the soil to directly measure soil water content and 205 thermal properties when the sensor is placed in the soil. The base rods were in contact 206 with the ceramic to measure ceramic thermal properties, water content and electrical 207 conductivity. The ceramic matric potential was estimated using the pre-determined 208 calibration curve  $(\lambda - \psi_m, C - \psi_m, \theta - \psi_m \text{ or } \sigma - \psi_m)$ . Depending on different measurement 209 environments, the various calibration curves proposed in this study can be selected to 210 achieve the highest prediction accuracy of matric potential. The measured ceramic 211 matric potential was equal to the soil matric potential when both of them are at 212 equilibrium.

229

The following two sections focus on the sensor optimization in terms of soilceramic equilibrium and meanwhile considering the effects of heat transfer for DPHP measurements (Section 2.2) and electromagnetic transport for TDR measurements (Section 2.3) with COMSOL simulations. Different scenarios were tested and literature data were used for verification and validation.

# 218 2.2 COMSOL simulation of heat transport with heat pulse method

#### 219 2.2.1. Numerical model setup and governing equations

220 An optimal ceramic should be small to ensure faster water equilibration and prevent excessive soil disturbance. However, a too small ceramic radius ( $R_C$ , mm) 221 222 leads to heat loss from the ceramic in the radial direction, and a too short ceramic 223 length ( $L_C$ , mm) leads to the measured temperature rise released by the heat pulse method being affected by the axial heat transfer at the interface between the two 224 225 mediums. A 2D axisymmetric model of module of heat transfer in solids in COMSOL 226 (Version 6.1, COMSOL, Inc., Burlington, MA, USA) was used to optimize the sensor 227 size based on the module of heat transfer in solids. The governing equation used in the 228 module is:

$$C\frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + Q \quad t > 0 \tag{3}$$

where *t* is time (s), *Q* is rate per unit volume of heat generation for the numerical model (W m<sup>-3</sup>). Assuming that the heat is uniformly distributed in the heater of heat pulse, then in the heater volume, *Q* can be represented by:

233 
$$Q = \begin{cases} q' S_H & 0 < t \le t_0 \\ 0 & t > t_0 \end{cases}$$
(4)

where  $S_H$  is the cross-sectional area of the heater (m<sup>2</sup>),  $t_0$  is the heat pulse duration (s). For a linear heat source, *d* is negligible, i.e.,  $S_H$  approaches 0.

As shown in Figure 2a, soil, ceramic and handle were represented by rectangles
with dimensions of 80 mm width × 200 mm height, 30 mm width × 65 mm height and

238 30 mm width  $\times$  65 mm height, respectively. Note that  $L_C$  and  $R_C$  could be modified in 239 subsequent tests. To simplify the model, the heater and the temperature-sensing rods 240 were not shown in the figure. A linear heat source was added on the axis of symmetry. 241 The linear heat source was 140 mm in length, of which 10 mm was in the lower end 242 of the handle, 65 mm was distributed throughout the ceramic and the remaining 65 243 mm was in the soil. The length of the heat source in the ceramic and the soil could be 244 modified with the  $L_C$  and the length of the extended rod buried in soil ( $L_S$ , mm) in the 245 subsequent simulation. The distance between the domain point probe and the linear 246 heat source was 6 mm, corresponding to the rod spacing of 6 mm. The temperature 247 rise curves of the ceramic and the soil were obtained using domain point probes. The 248 outer boundary of the entire study region was set to thermal insulation. This boundary condition indicates that the heat flowing across the outer boundary is negligible. This 249 setting is reasonable because a sufficiently large area is chosen for analysis to 250 251 conform to the assumption of the infinite measured medium in the ILS model. The material properties of the handle were set to  $\lambda = 0.36$  W m<sup>-1</sup> °C<sup>-1</sup>; density,  $\rho = 1410$ 252 kg m<sup>-3</sup>; and specific heat,  $c = 1286 \text{ J kg}^{-1} \text{ °C}^{-1}$  (Kamai and Hopmans 2007). The setup 253 254 of material properties for ceramic and soil are described in detail in Section 2.2.3. 255 Since the mesh resolution affects simulation accuracy, we established a maximum 256 mesh size of 0.92 mm in the ceramic region and the region between the heater and the 257 temperature-sensing rod. The maximum mesh size for the other regions increased 258 from 0.92 mm to 2.3 mm based on a maximum element growth rate of 1.1 (Figure 2a). To generate easier identification of the maximum temperature rise and avoid 259 260 convective heat transfer around the heater, Kluitenberg (2002) suggested maximum 261 temperature rise should fall in the range of 0.5–1.5 °C. Based on this, by testing the 262 ceramic and soil with different water content, the optimal q' and  $t_0$  were determined to be 58 W  $m^{-1}$  and 8 s, respectively. 263



264

Figure 2. The scenario and the mesh for (a) heat pulse numerical simulation (the mesh area wasnot completely drawn) and (b) TDR sensitivity simulation.

# 267 **2.2.2. Verification of heat pulse simulation**

268 The validity of heat pulse simulation were verified based on the experimental 269 setup and measured data of Mori et al. (2003) and Kluitenberg et al. (2010). The 270 thermal properties of dry sand, water and saturated sand measured by heat pulse were 271 simulated by adjusting the sensor setup and the material properties of the measured medium. In <u>Kluitenberg et al. (2010)</u>, the L of the sensor was 27 mm, and the r was 272 273 4.99, 5.81 and 6.66 mm, corresponding to the rods subjected to inward deflection, no deflection, and outward deflection, respectively. Applied q' was 110 W m<sup>-1</sup> for  $t_0$  of 8 274 s. The  $\lambda$ ,  $\rho$  and specific heat c of the measured medium are shown in **Table 1**. 275

**Table 1.** *Material properties for simulation verification. Note that the symbol*  $\lambda$  *represents thermal conductivity,*  $\rho$  *represents wet bulk density, and c represents specific heat.* 

Medium	Deflection treatment	$\lambda (W m^{-1} \circ C^{-1})$	ho (kg m <sup>-3</sup> )	$c (\mathrm{J \ kg}^{-1} \ ^{\circ}\mathrm{C}^{-1})$
	inward	0.26	1630	759
Dry sand	none	0.26	1630	759
	outward	0.29	1630	759
	inward	0.6	998	4182
Water	none	0.6	998	4182
	outward	0.59	998	4182

	inward	1.85	2000	1393
Saturated sand	none	1.85	2000	1393
	outward	1.89	2000	1393

#### 278 **2.2.3.** Material properties for heat pulse simulations

279 Measurement using the multifunctional sensor requires that water in ceramic 280 equilibrates with soil water, but this does not mean that the water contents of the two 281 mediums are equal, and the water content gradient may change due to the surrounding 282 soil. To broaden the applicability of the simulation, 36 water content combinations 283 were considered, i.e., six degrees of saturation ranging from dry to saturation (the 284 water content at saturation is equal to total porosity) were set to ceramic and soil, 285 respectively. The degrees of saturation or water contents of the medium was numerically reflected by  $\lambda$ , c and  $\rho$ . The thermal conductivity and specific heat of 286 287 ceramic corresponding to different water contents were measured by a thermo-TDR 288 and the wet bulk density of ceramic was measured by weighing. The sandy soil 289 provided by Kodešová et al. (2013), which had a wide range of thermal conductivity, 290 was used as the simulated soil. The sandy soil comprised of 93.7% sand, 3% silt, and 3.3% clay, with  $\rho = 1710$  kg m<sup>-3</sup>, porosity (p) of 0.396 and volumetric heat capacity 291 of solids ( $\rho_{solids}c_{solids}$ ), of 2.164 M J m<sup>3</sup> °C<sup>-1</sup>. 292

The thermal conductivity corresponding to different soil water contents was predicted based on the <u>Yan et al. (2019)</u> model:

295 
$$\lambda = \begin{cases} \lambda_{dry} & \theta \le 0.01 \\ \left(\lambda_{sat} - \lambda_{dry}\right) \frac{1 + \left(\frac{p}{\beta}\right)^{-\beta}}{1 + \left(\frac{\theta}{\beta}\right)^{-\beta}} + \lambda_{dry} & \theta > 0.01 \end{cases}$$
(5)

where  $\lambda_{dry}$  and  $\lambda_{sat}$  are dry and saturated thermal conductivity, respectively (W m<sup>-1</sup> °C<sup>-1</sup>);  $\beta$  is empirical parameter;  $\lambda_{dry}$  was calculated by the linear function proposed by <u>He et al. (2017)</u>:

299 
$$\lambda_{dry} = -0.5815 p + 0.4999 \quad p \le 0.86$$
 (6)

300  $\lambda_{sat}$  was calculated by the geometric mean model proposed by <u>Woodside and</u>

301 <u>Messmer (1961)</u>:

302

$$\lambda_{sat} = \lambda_w^p \lambda_{solids}^{1-p} \tag{7}$$

303 where  $\lambda_w$  is the thermal conductivity of water, which is 0.594 W m<sup>-1</sup> °C<sup>-1</sup> at 20 °C 304 (Bristow 2002),  $\lambda_{solids}$  is the thermal conductivity of solids, which can be determined 305 by another geometric mean model based on the thermal conductivity and mass 306 fractions of quartz and other minerals (Johansen 1975; He et al. 2020):

307 
$$\lambda_{solids} = \lambda_q^{qc} \lambda_o^{1-qc}$$
(8)

where qc is quartz content,  $\lambda_q$  is thermal conductivity of quartz (7.7 W m<sup>-1</sup> °C<sup>-1</sup>), and  $\lambda_o$  is thermal conductivity of other minerals, which is assumed to be 2.0 W m<sup>-1</sup> °C<sup>-1</sup> and 3.0 W m<sup>-1</sup> °C<sup>-1</sup> for soils with qc > 20% and  $qc \le 20\%$ , respectively. Similar to <u>Peters-Lidard et al. (1998), Lu et al. (2007)</u> and <u>He et al. (2020)</u>, quartz content was assumed to be equal to the sand content. According to <u>Yan et al. (2019)</u>,  $\beta$  was calculated based on the sand fraction for soil solids ( $f_{sa}$ , gravimetric %):

314 
$$\beta = -0.303\lambda_{sat} - 0.201f_{sa} + 1.532 \tag{9}$$

315 And the  $\rho$  of the soil was predicted based on  $\rho_b$  and  $\theta$ , written as:

316  $\rho = \rho_b + \theta \rho_w \tag{10}$ 

317 where  $\rho_w$  is the density of water (1000 kg m<sup>-3</sup>). The *c* of the soil was calculated as:

 $c = C / \rho \tag{11}$ 

319 where the *C* of soil was predicted from the volumetric heat capacity of soil solids and 320 water:

321 
$$C = (1 - p)\rho_{solids}c_{solids} + \theta\rho_w c_w$$
(12)

where  $c_w$  is the specific heat of water (4180 J kg<sup>-1</sup> °C<sup>-1</sup>). The soil physical properties corresponding to saturation degrees (i.e., ratio of water content to saturated water content) of 0, 0.2, 0.4, 0.6, 0.8, 1.0 were used. The material properties of ceramic and soil are shown in **Table 2**.

The effect of  $R_C$ ,  $L_C$  and  $L_S$  on the measurements were studied by changing the basic sensor dimension in Section 2.1. Only one effect was assessed in each

simulation to avoid complications from additional effects. The ceramic temperature rise with 8  $R_C$  gradients (9, 12, 15, 18, 21, 24, 27 and 30 mm) and 36 water content combinations (288 treatments) was simulated. Ceramic thermal conductivity ( $\lambda_C$ ) was estimated based on the pulsed infinite line source model, which was used to screen the optimal  $R_C$ . The optimal  $R_C$  was used to optimize  $L_C$ , with the  $L_C$  set to 30, 35, 40, 45, 50, 55, 60 and 65 mm. Similarly, the optimization results were used to optimize  $L_S$ , and the settings of  $L_S$  and  $L_C$  were consistent.

**Table 2.** *Material properties of the ceramic and soil for simulations. Note that the symbol*  $\lambda$  *represents thermal conductivity,*  $\rho$  *represents wet bulk density,* and *c represents specific heat.* 

1	<i>V I</i>	, I	1 5
Medium	$\lambda (W m^{-1} °C^{-1})$	ho (kg m <sup>-3</sup> )	$c (J kg^{-1} °C^{-1})$
Dry ceramic	0.35	951	1049
Unsaturation ceramic 1	0.53	1071	1472
Unsaturation ceramic 2	0.61	1192	1668
Unsaturation ceramic 3	0.74	1278	1802
Unsaturation ceramic 4	0.95	1311	2037
Saturation ceramic	1.37	1427	2093
Dry soil	0.27	1710	764
Unsaturation soil 1	1.63	1789	916
Unsaturation soil 2	2.04	1868	1054
Unsaturation soil 3	2.30	1948	1181
Unsaturation soil 4	2.50	2027	1298
Saturation soil	2.65	2106	1407

# 337 2.3 COMSOL simulations of TDR-measured dielectric permittivity and electrical

#### 339 2.3.1. Theory for measurement sensitivity of TDR

Ignoring the effect on the measurements of the heterogeneity of dielectric permittivity in the plane parallel to the rods, the effective dielectric permittivity ( $\varepsilon_{eff}$ ) and effective electrical conductivity ( $\sigma_{eff}$ ) can be predicted by the sensitivity of TDR rods to lateral variations in dielectric permittivity (Knight 1992; Ferré et al. 2003; Nissen et al. 2003). The spatial weighting factor w(x, y) is the energy proportion of a specific point in the heterogeneous medium field with the same boundary conditions.

<sup>338</sup> conductivity

346 The w(x, y) at each point for the spatial sensitivity of the TDR rod is defined as:

347 
$$w(x, y) = \frac{\left|\nabla\Phi(x, y)\right|^2}{\iint_{\Omega} \left|\nabla\Phi_0(x, y)\right|^2 dx dy}$$
(13)

348 where  $\nabla \Phi(x, y)$  and  $\nabla \Phi_0(x, y)$  are potential gradients in homogeneous and 349 heterogeneous fields (V m<sup>-1</sup>), respectively. The  $\nabla \Phi(x, y)$  satisfies:

350 
$$\nabla \Phi(x, y) = -E(x, y) \tag{14}$$

351 where E(x, y) is the electric field intensity (V m<sup>-1</sup>) and could be computed using 352 COMSOL. The weighting function is defined as:

353 
$$\iint_{\Omega} w(x, y) dx dy = 1$$
(15)

354  $\varepsilon_{eff}$  and  $\sigma_{eff}$  are calculated as:

355 
$$\varepsilon_{eff} = \iint_{\Omega} \varepsilon(x, y) w(x, y) dx dy$$
(16)

356 
$$\sigma_{eff} = \iint_{\Omega} \sigma(x, y) w(x, y) dx dy$$
(17)

357 The contribution level of the measured medium (ceramic) to  $\varepsilon_{eff}$  is expressed as the 358 measurement sensitivity to the ceramic of the TDR (*MSC*):

$$MSC = \iint_C w_C(x, y) dx dy$$
(18)

360 where  $w_C(x, y)$  is the weighting factor that is distributed in the ceramic region. 361 Similarly, the measurement sensitivity to the soil surrounding the ceramic of the TDR 362 (*MSS*) is:

363 
$$MSS = \iint_{S} w_{S}(x, y) dx dy$$
(19)

364 where  $w_S(x, y)$  is the weighting factor that is distributed in the soil region. In a plane 365 perpendicular to the TDR rods, *MST* and *MMS* satisfy:

$$366 \qquad MSC + MSS = 1 \tag{20}$$

367 The effective ceramic dielectric permittivity ( $\varepsilon_{eff-C}$ ) and effective ceramic electrical 368 conductivity ( $\sigma_{eff-C}$ ) measured by TDR can be expressed as:

$$\mathcal{E}_{eff-C} = MSC \times \mathcal{E}_{C} + MSS \times \mathcal{E}_{S}$$
(21)

$$\sigma_{eff-C} = MSC \times \sigma_{c} + MSS \times \sigma_{s}$$
<sup>(22)</sup>

371 where  $\varepsilon_C$  and  $\varepsilon_S$  are the apparent dielectric permittivity of ceramic and soil, 372 respectively, and  $\sigma_C$ ,  $\sigma_S$ , are the apparent electrical conductivity of ceramic and soil, 373 respectively. Therefore, a greater value of the *MSC* for TDR indicates a larger 374 sensitivity to the ceramic and a higher accuracy.

# 375 **2.3.2.** Simulation setup in the module of alternating current/direct current

376 The ceramic radius in terms of electromagnetic propagation was optimized by 377 using the alternating current/direct current (AC/DC) module of COMSOL. A 2D 378 model was established to simulate the electrostatic field perpendicular to the plane of 379 the TDR rods. As shown in Figure 2b, the central rod of the TDR, ceramic and soil 380 surrounding ceramic were represented by circles with radii of 0.6, 7 (adjustable) and 381 40 mm, respectively. At 6 mm to the left and to the right of the central rod, two circles 382 with a radius of 0.6 mm were added to represent the outer rods. The entities of the 383 three smallest circles are subtracted to simplify the model. The initial value of the 384 entire study region was set to 0. Similar to Bruvik et al. (2012) and Zhan et al. (2015), 385 the outer boundary of the soil and the two outer rods was set as zero charge and 386 ground boundary conditions, respectively, and the central rod was set as terminal 387 boundary condition, with the type voltage and the value of 1. Different combinations 388 of ceramic radius and dielectric permittivity were set by parametric sweep to yield different electrostatic fields. The ceramic dielectric permittivity was set to 3, 6, 9, 12, 389 390 15, and 19, as measured by a TDR. The ceramic dielectric permittivity was set to 2, 5, 391 10, 15, 20, and 25, corresponding to the soil water content from drying to saturation 392 (Nissen et al. 2003; Lekshmi et al. 2014). The ceramic radius increased from 7 to 18 393 mm in steps of 0.1 mm. Therefore, 3960 ( $6 \times 6 \times 110$ ) treatments were set. The mesh 394 used was the smallest mesh by default (0.0016-0.8 mm).

The matric potential sensor based on the relationship between the ressistance and matric potential fails when the electrical conductivity is higher than 0.5 dS m<sup>-1</sup> (<u>Campbell and Gee 1986; Xin et al. 2007</u>). Therefore, the electrical conductivity set in this study ranged from 0.01 to 0.50 dS m<sup>-1</sup>. In addition, the electrical conductivity is 399 related to the water content, that is, there is a certain correlation between the electrical 400 conductivity and the dielectric permittivity (Hamed et al. 2003; Kargas and Soulis 401 2019). Consequently, 54 electrical conductivity combinations based on low, medium 402 and high water contents were considered (Table 3). The ceramic radius increased 403 from 7 to 18 mm in steps of 0.1 mm. Therefore, 5940 ( $54 \times 110$ ) treatments were set. 404 Based on the computed electric field intensity and the given dielectric permittivity and 405 electrical conductivity,  $\varepsilon_{eff-C}$  and  $\sigma_{eff-C}$  were determined using Equation (21) and (22), 406 respectively.

407 **Table 3.** Ceramic-soil electrical conductivity combinations based on low, medium and high water 408 contents. Note that the symbol  $\varepsilon_C$  represents apparent dielectric permittivity of ceramic,  $\sigma_C$ 409 represents apparent electrical conductivity of ceramic,  $\varepsilon_S$  represents apparent dielectric 410 permittivity of soil,  $\sigma_S$  represents apparent electrical conductivity of soil.

Water content treatment	$\varepsilon_C$	$\sigma_C (\mathrm{dS m}^{-1})$		$\varepsilon_C \qquad \sigma_C (\mathrm{dS \ m}^{-1}) \qquad \varepsilon_S$		s	$\sigma_{S} (\mathrm{dS m}^{-1})$		
low water content	3	0.01	0.02	0.03	2	5	0.01	0.02	0.03
medium water content	2	0.04	0.12	0.20	10	15	0.04	0.12	0.20
high water content	9	0.10	0.30	0.50	20	25	0.10	0.30	0.50

#### 411 **2.3.3. Verification for TDR sensitivity simulation**

412 The validity of TDR sensitivity simulation was verified based on the 413 experimental setup and measured data of Nissen et al. (2003). The effect of fluid level 414 height on the  $\varepsilon_{eff}$  measurements were simulated and analyzed with a horizontally 415 placed TDR. The study region was expanded to a square with a side length of 300 416 mm, and the medium boundary was adjusted to a horizontal line to represent the liquid-air interface. The bottom material was set as ethanol or water, corresponding to 417 418 the dielectric permittivity of 25 and 80 respectively. The top boundary material was 419 set as air, corresponding to the dielectric permittivity of 1. The rod radius and spacing 420 were adjusted to 2.3 mm and 35 mm respectively. The simulation results were 421 compared with the measurements.

#### 422 **2.4 Statistical analysis**

423 The estimated physical properties based on COMSOL simulation ( $x_{eff}$ ) were 424 normalized:

425 
$$x_n = \frac{x_{eff}}{x}$$
(23)

426 where  $x_n$  and x represent the normalized physical properties and the known reference 427 values as preset for the medium in the simulation, respectively. Likewise, the absolute 428 value of relative error ( $RE_a$ ) was calculated to evaluate the influence of different 429 sensor sizes on the accuracy:

430 
$$RE_a = \left| \frac{x_{eff} - x}{x} \times 100\% \right|$$
(24)

Root means square error (*RMSE*) was used to compare the simulated temperature risedata with the measured data in the literatures:

433 
$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (x_s - x_m)^2}{n}}$$
(25)

434 where  $x_s$  and  $x_m$  represent the simulated data based on COMSOL and measured data in 435 the literatures, respectively, and *n* is the number of data points. To match the 436 simulated data, the measure data were modified by using an interpolation function in 437 Matlab.

# 438 **3 Results and discussion**

#### 439 **3.1 Simulation verification**

## 440 **3.1.1. Verification for heat pulse simulation**

441 The temperature rise curves of DHPP heated water, dry sand and saturated sand 442 were simulated and compared with the measurements of Kluitenberg et al. (2010). As 443 shown in Figure 3, the simulated temperature rise curves were in good agreement 444 with the measurements. However, the interference of many uncontrollable factors in 445 the measurement leaded to error, including the thermal resistance of the contact 446 between the rods and the dry sand for the dry sand cases. In the case of outward deflected rods for measuring saturated sand, the *RMSE* was  $7.29 \times 10^{-3}$  °C, which was 447 the lowest, while in the case of outward deflected rods for measuring dry sand, the 448 *RMSE* was  $1.60 \times 10^{-1}$  °C, which was the greatest. Even though, the *RMSE* were 449

450 within an acceptable range, which indicated that our COMSOL models were accurate

451 and can be applied to the sensor optimization.



452

453 Figure 3. Measured (M) and simulated (S) temperature rise curves of dry sand, water, and 454 saturated sand. All results were for the same DPHP sensor, with rods subjected to inward 455 deflection (I), no deflection (N), and outward deflection (O). Measurements were retrieved from 456 Mori et al. (2003) and Kluitenberg et al. (2010).

# 457 **3.1.2. Verification of TDR sensitivity simulation**

By comparing the dielectric permittivity measured by <u>Nissen et al. (2003)</u> at different liquid levels with our COMSOL simulation results, the feasibility of using COMSOL simulation to study TDR sensitivity was examined. The results of measurement and simulation are shown in **Figure 4**. The simulations deviated from the measurements when the air-liquid boundary was at close proximity to the rod midpoint, although their trends were similar. The *RMSE* values were as low as  $2.43 \times 10^{-3}$  and  $3.99 \times 10^{-3}$  for water and ethanol, respectively. Therefore, our simulation can accurately and reliably predict TDR sensitivity and evaluate sensor accuracy.



466

Figure 4. Measured (M) and simulated (S) normalized dielectric permittivity ( $\varepsilon_n$ ) of water and ethanol for the air-liquid interface at difference distances related to the rod midpoint (0 indicates the air-liquid interface is located at the rod midpoint, positive and negative values indicate interface is above and below the rod midpoint, respectively). Data were retrieved from <u>Nissen et</u> al. (2003).

# 472 **3.2** Simulation for thermal property estimations

#### 473 **3.2.1** Ceramic radius optimization for simulating thermal conductivity

474 The widely used ILS model is based on the assumption that the heat pulse 475 sensors are embedded in an infinite and homogenous medium (Campbell et al. 1991; 476 Philip and Kluitenberg 1999). The medium heterogeneity affects the heat transfer process, and therefore changes the temperature field, heat flux and temperature rise 477 478 curve (Ren et al. 2005). The simulation results of temperature field and heat flux 479 corresponding to different ceramic radii are shown in Figure 5. The porous ceramic 480 matrix with a larger radius can retain more energy released by the heat pulse. 481 Therefore, less of the heat propagates to the surrounding soil through radial heat 482 transfer, which leads to lower estimation error. Figure 6 shows the simulated ceramic 483 temperature rise curves (i.e., temperature as a function of time) based on different 484 combinations of thermal properties of ceramic and soil. The ceramic temperature rises 485 shown in Figure 6d and 6g were higher due to the higher C caused by the higher 486 ceramic water content, while in other cases the result was opposite due to the lower 487 ceramic water content. When the ceramic radius was 9 mm, the temperature rise 488 curves deviated noticeably. With the increase in ceramic radius, the deviation of the 489 temperature rise curves decreased until they tended to be constant. In addition, the 490 deviation degree of the temperature rise curves was affected by the difference in 491 thermal properties between the two mediums. As shown in Figure 6a and 6h, the 492 temperature rise curves deviated slightly due to the similarity of the thermal properties 493 of soil and ceramic. On the contrary, the considerable difference in thermal properties 494 between the soil and ceramic increased the difficulty of obtaining accurate 495 temperature rise curves, such as Figure 6c and 6g. For these cases, the ceramic radius 496 must be increased to improve the estimation accuracy.

497 **Figure 7** shows the normalized ceramic thermal conductivity  $(\lambda_{n-C})$ corresponding to 36 combinations of thermal properties. The  $\lambda_{n-C}$  is inaccurate 498 499 because it is based on both the ceramic and the soil when the ceramic cross section is 500 smaller than the sampling area of the heat pulse. The positive or negative relative 501 error dependeds on the difference in thermal properties between the ceramic and the 502 soil, which is in agreement with Figure 6. Estimation accuracy improved with increasing ceramic radius. The  $\lambda_{n-C}$  was between 0.99 and 1.01 when the ceramic 503 504 radius  $\geq 18 \text{ mm}$  (Figure 7), which indicates that the *RE<sub>a</sub>* caused by radial heat transfer 505 can be controlled within 1% when the ceramic radius is 18 mm. The theoretical 506 analysis of Campbell et al. (1991) showed that at the time corresponding to the 507 maximum temperature rise, the outer boundary with a temperature rise of 1% of the 508 maximum temperature rise was a circle with a radius of 2.37 r. The results of Ren et 509 al. (2005) indicated that the sampling area of the heat pulse was a circle with a radius 510 of 14 mm, i.e., 2.3 r. Thus, the optimal ceramic radius is larger than the theoretical 511 analysis and experimental results. This may be attributed to that considerable 512 difference in thermal properties between the soil and the ceramic are considered in our 513 study. It should be noted that, in practice, the water contents of the ceramic and the 514 soil are similar due to water equilibration, i.e., there are few cases where the thermal 515 properties of the two mediums are noticeably different. Therefore, the ceramic radius 516 of 18 mm can ensure high accuracy of the sensor ( $RE_a < 1\%$ ).



517

**Figure 5.** COMSOL simulated temperature distribution and heat flux at ceramic radius,  $R_C = 9$ , 12, 15, 18, 21, 24, 27 and 30 mm at 180 s after the 8-s heat input when ceramic thermal conductivity,  $\lambda_C = 0.35$  W m<sup>-1</sup> °C<sup>-1</sup> and soil thermal conductivity,  $\lambda_s = 2.65$  W m<sup>-1</sup> °C<sup>-1</sup>. Arrow direction represents direction of heat transfer, arrow size is proportional to magnitude of heat flux.



**Figure 6.** COMSOL simulated ceramic temperature rise as a function of time for different combinations of thermal conductivity of ceramic and soil. Ceramic thermal conductivity,  $\lambda_C$  that is set to be 0.35, 0.61 and 1.37 W m<sup>-1</sup> °C<sup>-1</sup> and soil thermal conductivity,  $\lambda_S$  that is set to be 0.27, 2.04, and 2.65 W m<sup>-1</sup> °C<sup>-1</sup>; ceramic radius ranged from 9 to 30 mm. The data following  $\lambda_C$  or  $\lambda_S$  is the value of thermal conductivity (W m<sup>-1</sup> °C<sup>-1</sup>).



526

**Figure 7.** Normalized ceramic thermal conductivity  $(\lambda_{n-C})$  as related to different ceramic radius ( $R_C$ , with the settings of 9, 12, 15, 18, 21, 24, 27 and 30 mm) for different combinations of thermal conductivity of ceramic ( $\lambda_C$ , ranging from 0.35 to 1.37 W m<sup>-1</sup> °C<sup>-1</sup>) and soil ( $\lambda_S$ , ranging from 0.27 to 2.65 W m<sup>-1</sup> °C<sup>-1</sup>), the unoptimized ceramic length and extended rod length is set to be 65 mm. The data following  $\lambda_C$  or  $\lambda_S$  is the value of thermal conductivity (W m<sup>-1</sup> °C<sup>-1</sup>), and the regions with the absolute value of relative error ( $RE_a$ ) < 1% are marked with gray rectangle.

533

#### **3.2.2** Ceramic length optimization for simulating thermal conductivity

Figure 8 shows the results of the  $\lambda_{n-C}$  corresponding to the 36 thermal property combinations, with all results based on the ceramic radius of 18 mm. The error caused by axial heat transfer decreased and the accuracy of thermal conductivity estimation improved with increasing ceramic length. Some extreme cases were excluded, such as soil thermal conductivity ( $\lambda_s$ ) higher than 2.04 W m<sup>-1</sup> in Figure 8a and  $\lambda_s$  of 0.27 W

 $m^{-1}$  in Figure 8f, because they represent the assumption that one medium is dry and 539 540 the other medium is at a higher water content. Based on this, we found that the  $\lambda_{n-C}$ was between 0.98 and 1.02 when the ceramic length  $\geq$  40 mm (as shown in the area 541 542 marked by the gray rectangle in Figure 8), i.e., the  $RE_a$  caused by axial heat transfer can be controlled within 2%. Axial heat conduction occurred not only between the 543 544 ceramic and the soil, but also between the handle and the soil. Meng et al. (2023) 545 indicated that accurate measurement of thermal properties became more challenging 546 as thermal properties of handle material increase relative to those of the measured medium. Therefore, the overestimation or underestimation of the  $\lambda_C$  did not 547 completely correspond to the higher or lower  $\lambda_S$ , and the effect from the handle needs 548 549 to be additionally considered. For example, in the case of Figure 8f where  $\lambda_S$  was 550 higher than that of the ceramic, the  $\lambda_C$  may be underestimated, because of the large 551 difference in thermal conductivity between the ceramic and the handle (the handle thermal conductivity was only 0.36 W m<sup>-1</sup>). For the case in Figure 8a where the  $\lambda_s$ 552 was  $0.27 \text{ W m}^{-1}$ , the temperature rise of the handle was less than that of the ceramic 553 due to the high heat capacity of the handle and the short (10 mm) heat source in the 554 555 handle. Due to the temperature gradient, more heat in the ceramic was transferred to the handle, which led to an overestimation of the  $\lambda_C$ . 556



**Figure 8.** Normalized ceramic thermal conductivity  $(\lambda_{n-C})$  as related to different ceramic lengths ( $L_C$ , with the settings of 30, 35, 40, 45, 50, 55, 60 and 65 mm) for different combinations of thermal conductivity of ceramic ( $\lambda_C$ , ranging from 0.35 to 1.37 W m<sup>-1</sup> °C<sup>-1</sup>) and soil ( $\lambda_S$ , ranging from 0.27 to 2.65 W m<sup>-1</sup> °C<sup>-1</sup>), the optimized ceramic radius and unoptimized extended rod length were set to 18 mm and 65 mm, respectively. The data following  $\lambda_C$  or  $\lambda_S$  is the value of thermal conductivity (W m<sup>-1</sup> °C<sup>-1</sup>), and the regions with the absolute value of relative error ( $RE_a$ ) < 2% are marked with gray rectangle.

557

#### 565 **3.2.3 Optimization of the extended rod length for simulating thermal conductivity**

The extended rod length was optimized based on the optimal ceramic radius and length. The relationship between normalized soil thermal conductivity ( $\lambda_{n-S}$ ) and the extended rod length is shown in **Figure 9**. The accuracy of  $\lambda_S$  estimation improved with increasing extended rod length due to a decrease in the error caused by axial heat 570 transfer. However, considering the deflection problem caused by the long rods, the 571 extended rod length of 50 mm was finally adopted. At the 50-mm extended rod 572 length, the  $RE_a$  of  $\lambda_s$  estimation was less than 3% as shown in the regions marked by 573 the gray rectangles in **Figure 9**, which was 3% lower than that of a traditional thermo-574 TDR with rod length of 40 mm (He et al. 2018). Therefore, our optimization 575 considerably improved the sensor accuracy.





**Figure 9.** Normalized soil thermal conductivity  $(\lambda_{n-S})$  as related to different extended rod length  $(L_S, \text{ with the settings of 30, 35, 40, 45, 50, 55, 60 and 65 mm) for different combinations of thermal conductivity of ceramic <math>(\lambda_C, \text{ ranging from 0.35 to 1.37 W m}^{-1} \circ \text{C}^{-1})$  and soil  $(\lambda_S, \text{ ranging from 0.27 to 2.65 W m}^{-1} \circ \text{C}^{-1})$ , the optimized ceramic radius and length were set to 18 mm and 40 mm, respectively. The data following  $\lambda_C$  or  $\lambda_S$  is the value of thermal conductivity (W m}^{-1} \circ \text{C}^{-1}), and the regions with the absolute value of relative error  $(RE_a) < 3\%$  are marked with gray rectangle.

For the cases of  $\lambda_s = 0.27 \text{ W m}^{-1} \circ \text{C}^{-1}$ , the *RE*<sub>a</sub>s are lower than others as shown in 584 585 **Figure 9a**. The explanation may be that less heat was lost from the soil with low  $\lambda_S$  to the surrounding medium during the temperature measurement, which resulted in a 586 587 smaller area of the soil affected by heat pulse. Unlike the ceramic optimization results, 588 the estimated errors were all positive, even if the  $\lambda_S$  was much lower than  $\lambda_C$ . This is 589 because the  $\lambda_S$  estimation is not only affected by the difference in thermal conductivity 590 between the two mediums, but also by the finite length of the heat source, and the 591 latter always contributes a positive error (Kluitenberg et al. 1993). Therefore, longer 592 extended rods will not only reduce the influence of medium heterogeneity on the 593 temperature measuring point, but also avoid deviation from the assumption of the heat 594 source of finite length. However, it is also noteworthy that long rods would be 595 affected by deflection when inserting into soils and significantly affect measurement 596 accuracy (Kluitenberg et al. 1993; Bristow et al. 1994; Kluitenberg et al. 1995).

597 The relative location of the temperature measuring point was defined as the ratio of the distance from the temperature measuring point to the ceramic-soil boundary (D, 598 599 mm) to the extended rod length. The effect of the evaluated rod length and the relative 600 location of the temperature measuring point on the estimation of  $\lambda s$  was evaluated, 601 and the results were shown in Figure 10. In the simulations, ceramic was represented 602 as soils (corresponding to the cases represented by dotted lines in Figure 10) to 603 exclude the effect of heterogeneity and evaluate the effect of the heat source of finite 604 length on the estimations. The results indicated that the positive error caused by heat 605 source of finite length increased with increasing value of  $D/L_s$ . The  $\lambda_n$ -s showed a 606 stable trend because the positive error caused by heterogeneity decreased with 607 increasing value of  $D/L_{\rm S}$  (Figure 10a). While the  $\lambda_n$ -s showed an increasing trend 608 because the negative error caused by heterogeneity decreased with increasing value of 609  $D/L_{\rm S}$  (Figure 10b). For The RE<sub>a</sub> of the  $\lambda s$  estimation was the lowest when  $D/L_{\rm S}$  =0.50, that is, the midpoint of the extended rode was the optimal temperature measuring 610 611 point (Figure 10a). While the  $RE_a$  of the  $\lambda s$  estimation was the lowest when  $D/L_s =$ 

612 0.49 (Figure 10b), that is, the location closer to the ceramic was the optimal 613 temperature measuring point. The  $RE_a$  of the  $\lambda$ s estimation can be controlled within 614 1.5% and 0.2% by extended rod length of 50 mm and 80 mm, respectively, that is, the 615  $RE_a$  can be effectively reduced by increasing extended rod length, which is consistent 616 with the result in Figure 9.



617

618 **Figure 10.** Normalized soil thermal conductivity  $(\lambda_{n,S})$  related to the ratio of the distance from the 619 temperature measuring point to the ceramic-soil boundary (D, mm) to the extended rod length ( $L_s$ , 620 with the settings at 30, 40, 50 and 80 mm) for different combinations of thermal conductivity of ceramic ( $\lambda_c$ , with the settings of 0.35 and 1.37 W m<sup>-1</sup> °C<sup>-1</sup>) and soil ( $\lambda_s$ , with the settings of 0.27 621 and 2.65 W m<sup>-1</sup> °C<sup>-1</sup>), the optimized ceramic radius and length are set to 18 mm and 40 mm, 622 respectively. The data following  $\lambda_C$  or  $\lambda_S$  is the value of thermal conductivity (W m<sup>-1</sup> °C<sup>-1</sup>), and the 623 dotted lines represented cases in which the measured medium was homogeneous soil without 624 625 ceramic (Ho).

#### 626 **3.2.4 Estimation accuracy of volumetric heat capacity**

627 Figure 11 shows the normalized ceramic volumetric heat capacity  $(C_{n-C})$  and normalized soil volumetric heat capacity  $(C_{n-S})$  corresponding to the extreme thermal 628 property combinations. Compared with thermal conductivity, volumetric heat capacity 629 was more accurately estimated, even though the thermal properties of the ceramic and 630 631 soil differ greatly. This is consistent with numerical analysis of Philip and Kluitenberg (1999) and the experimental results of Zhang et al. (2014), which indicated that the 632 633 sensitivity of volumetric heat capacity data to heterogeneity is less than that of 634 thermal conductivity data to heterogeneity when near-surface STP were measured by



#### 636

637 Figure 11. (a) normalized ceramic volumetric heat capacity  $(C_{n-C})$  as related to ceramic radius 638  $(R_C)$ , the unoptimized ceramic length  $(L_C)$  and extended rod length  $(L_S)$  are set to be 65 mm; (b) 639  $C_{n-C}$  as related to  $L_C$ , the optimized  $R_C$  and unoptimized  $L_S$  are set to 18 mm and 65 mm, 640 respectively; and (c) normalized soil volumetric heat capacity  $(C_{n-S})$  as related to  $L_S$ , the optimized 641  $R_C$  and  $L_C$  are set to 18 mm and 40 mm, respectively, when different combinations of thermal conductivity of ceramic ( $\lambda_c$ , 0.35 and 1.37 W m<sup>-1</sup> °C<sup>-1</sup>) and soil ( $\lambda_s$ , 0.27 and 2.65 W m<sup>-1</sup> °C<sup>-1</sup>) 642 for. The data following  $\lambda_C$  or  $\lambda_S$  is the value of thermal conductivity (W m<sup>-1</sup> °C<sup>-1</sup>), and the regions 643 644 with the absolute value of relative error  $(RE_a) < 1\%$  are marked with gray rectangle.

The  $RE_a$  of estimated ceramic volumetric heat capacity caused by radial and axial heat transfer can be controlled within 1 % when the  $R_C \ge 15$  mm and  $L_C \ge 35$ mm, respectively. The  $RE_a$  of estimation of soil volumetric heat capacity caused by axial heat transfer and finite length of the heat source can be controlled within 1% 649 when  $L_S \ge 30$  mm. Similar to the soil thermal conductivity, the soil volumetric heat 650 capacity was always overestimated, which was also due to the limited length of the 651 heat source (Kluitenberg et al. 1993). Therefore, the optimized sensor sizes (ceramic 652 radius of 18 mm, ceramic length of 40 mm and extended rod length of 50 mm) based 653 on ceramic and soil thermal conductivity estimations can ensure a low  $RE_a$  (< 1%) of 654 ceramic and soil volumetric heat capacity estimation.

# 655 3.3 Simulations for the estimations of ceramic dielectric permittivity and 656 electrical conductivity

#### 657 **3.3.1** Ceramic radius optimization for dielectric permittivity estimations

Similar to thermal property estimation, the medium heterogeneity affects the 658 659 electric field, and therefore leads to errors in estimating dielectric permittivity and 660 electrical conductivity. The simulation results of electric field corresponding to 661 different ceramic radii are shown in Figure 12. The porous ceramic matrix with a 662 large radius can contain more energy released by the central rod. Therefore, less of the 663 energy prorogates to the surrounding soil and leads to lower estimation error. Figure 664 13 shows the results of ceramic radius optimization based on  $\varepsilon_C$  estimations. As 665 ceramic radius increased, normalized ceramic dielectric permittivity ( $\varepsilon_{n-C}$ ) gradually approached 1. The  $\varepsilon_{n-C}$  was between 0.99 and 1.01 when the ceramic radius  $\ge 13$  mm, 666 667 as shown in regions marked by the gray rectangles in Figure 13. The  $RE_a$  caused by 668 the difference in dielectric permittivity between the ceramic and the soil can be 669 controlled within 1% when the ceramic radius is 13 mm. The sampling radius of the 670 TDR with a rod diameter of 1.3 mm and a spacing of 6 mm is 11 mm, the associated 671  $RE_a$  of  $\varepsilon_C$  was 2%, which is in good agreement with <u>Ren et al. (2005)</u>.

A soil differing considerably in dielectric permittivity from the ceramic results in a higher  $\varepsilon_C$  estimations error. For example, the  $RE_a$ s of  $\varepsilon_C$  estimation at  $\varepsilon_S$  of 2 (blue hexagons), 5 (gray diamonds), 20 (green squares), and 25 (pink circles) at  $R_C = 7$  mm, were 11 %, 6 %, 2 %, and 3 %, respectively, which were higher than those of 1% at  $\varepsilon_S$ = 10 (orange triangles) and 15 (purple triangles) as indicated by Figure 13d. In 677 addition to the considerable dielectric permittivity difference between the two 678 mediums, a high  $RE_a$  may also be caused by a soil with a low dielectric permittivity. The  $RE_a$  of  $\varepsilon_C$  estimation at  $\varepsilon_S = 2$  (blue hexagons) was 7 % at  $R_C = 7$  mm, which was 679 680 higher than that of 3 % at  $\varepsilon_s = 25$  (pink circles), even though the dielectric permittivity of the two mediums were more similar in the former case as shown in Figure 13b. 681 Similarly, the  $RE_a$  of  $\varepsilon_C$  estimation at  $\varepsilon_S = 10$  (orange triangles) was 3 % at  $R_C = 7$ 682 mm, which was higher than that of 2% at  $\varepsilon_s = 25$  (pink circles) as shown in Figure 683 684 13a. This is because the measurement sensitivity is biased toward the lower 685 permittivity region, as the soil with lower dielectric permittivity shows a higher 686 contribution to  $\varepsilon_{eff}$ . This bias arises because the potential gradient of the energy through the region with low dielectric permittivity is much higher than that through 687 the region with high dielectric permittivity. This is also shown by the simulation 688 results in Figure 12a, 12b, and 12c, where some soil regions have higher electric field 689 690 intensity than the ceramic on the edge due to its their lower dielectric permittivity 691 although the soil is further away from the central rod than the ceramic. According to 692 Eq. (13), a high potential gradient means that the energy and the sensitivity is concentrated within the region with low dielectric permittivity (Nissen et al. 2003). 693 Numerical analysis indicates that the interference medium with low dielectric 694 695 permittivity has a greater impact on the measured dielectric permittivity than the 696 interference medium with high dielectric permittivity (Knight et al. 1997). Therefore, 697 the soil with low dielectric permittivity and a considerable difference from  $\varepsilon_C$  result in 698 a high  $RE_a$  of  $\varepsilon_C$  estimation. For example, the  $RE_a$  of  $\varepsilon_C$  estimation (12%) was the highest of all cases for  $\varepsilon_S = 2$  and  $R_C = 7$  mm (Figure 13f). 699





701Figure 12. The simulated electric field intensity at ceramic radius,  $R_C = 7, 9, 11, 13, 15$  and 17 mm for the case of ceramic dielectric permittivity of 19 and soil702dielectricpermittivityof2.Circlesrepresenttheceramic-soilboundary.



**Figure 13.** Normalized ceramic dielectric permittivity ( $\varepsilon_{n-C}$ ) as related to ceramic radius ( $R_C$ , ranging from 7 to 18 mm) for different combinations of ceramic dielectric permittivity ( $\varepsilon_C$ , ranging from 3 to 19) and soil dielectric permittivity ( $\varepsilon_S$ , ranging from 2 to 25). The data following  $\varepsilon_C$  or  $\varepsilon_S$  is the value of dielectric permittivity, and the regions with the absolute value of relative error ( $RE_a$ ) < 1% are marked with gray rectangle.

709 3.3.2 Ceramic radius optimization for electrical conductivity estimations

Figure 14 shows the relationship between normalized ceramic electrical conductivity ( $\sigma_{n-C}$ ) and ceramic radius. When the ceramic radius was small, the  $RE_a$  of  $\sigma_C$  estimation was high; conversely, the error decreased with increasing ceramic radius. The  $RE_a$  was controlled within 1% for a radius up to 14.8 mm, as shown in the and regions marked by the gray rectangles (**Figure 14**).

715 According to Eq. (22), the error source of  $\sigma_C$  estimation was similar to that for 716  $\varepsilon_C$ , including the difference in values between  $\varepsilon_C$  and  $\varepsilon_S$  and the contribution of soil to 717  $\varepsilon_{eff-C}$ . Since the contribution level of the soil to  $\sigma_{eff-C}$  was calculated based on the 718 dielectric permittivity of the two mediums,  $\sigma_{eff-C}$  was affected by the dielectric 719 permittivity of the two mediums as well as their electrical conductivity. In Figure 720 14g, due to the greater difference in electrical conductivity between the soil and the 721 ceramic, the  $RE_a$  of  $\sigma_C$  estimation at  $R_C = 7$  mm was 22% for  $\varepsilon_S = 20$  and  $\sigma_S = 0.50$ 722 (orange triangles), which was higher than 11% for  $\varepsilon_s = 20$  and  $\sigma_s = 0.30$  (gray 723 diamonds). Due to the lower  $\varepsilon_s$ , in the case of  $\varepsilon_s = 20$  and  $\sigma_s = 0.50$  (orange triangles) 724 in Figure 14, at  $R_C = 7$  mm, the  $RE_a$  of  $\sigma_C$  estimation of 22% is greater than that of 725 18% corresponding to the case of  $\varepsilon_s = 25$  and  $\sigma_s = 0.50$  (pink circles). Nissen et al. 726 (2001) and Ferré et al. (2003) indicated that the sensitivity of TDR to electrical 727 conductivity measurement was independent of the conductivity distribution of the 728 medium. This conclusion differs from ours is that the interfering medium was not soil in their study, but air with electrical conductivity of 0. In this case, the part of " $\sigma_S \times$ 729 MSS" in Eq. (22) is equal to 0, and  $\varepsilon_{eff-C}$  is only affected by the dielectric permittivity 730 731 distribution, independent of the electrical conductivity distribution. The  $\sigma_{n-C}$  is 732 therefore equal to the contribution level of the measured medium to  $\varepsilon_{eff-C}$ , i.e., MSC in 733 Eq. (18).



734

Figure 14. Normalized ceramic electrical conductivity ( $\sigma_{n-C}$ ) as related to ceramic radius ( $R_C$ , ranging from 7 to 18 mm) for different combinations of ceramic dielectric permittivity ( $\varepsilon_C = 3$ , 12, and 19), soil dielectric permittivity ( $\varepsilon_S = 2$  and 5), ceramic electrical conductivity ( $\sigma_C = 0.1$ , 0.3 and 0.5 dS m<sup>-1</sup>) and soil electrical conductivity ( $\sigma_S = 0.01$ , 0.02 and 0.03 dS m<sup>-1</sup>). The data following  $\varepsilon_C$  or  $\varepsilon_S$  is the value of dielectric permittivity, the data following  $\sigma_C$  or  $\sigma_S$  is the value of electrical conductivity (dS m<sup>-1</sup>), and the regions with the absolute value of relative error ( $RE_a$ ) < 1% are marked with gray rectangle.

#### 739 4 Conclusion

740 A multifunctional sensor was developed by coupling heat pulse, TDR and matric 741 potential sensors to simultaneously measure soil water content, matric potential and 742 thermal properties of the same soil sample. The soil water content and thermal 743 properties are measured directly by the rods extended out of the ceramics, while the 744 soil matric potential can be predicted indirectly based on the thermal conductivity, 745 volumetric heat capacity, water content or electrical conductivity of the porous 746 ceramic matrix. Compared with the measured data in the literatures, our COMSOL 747 models were verified to be able to accurately and reliably evaluate the sensor error 748 and optimize the sensor. The simulation results indicated that a high estimation 749 accuracy can be attained by increasing the size of the porous ceramic matrix, even in 750 the presence of considerable differences in physical properties between the soil and 751 the ceramic matrix. Our optimization results indicate that the optimal design for the 752 porous ceramic matrix was a cylinder with a radius of 18 mm and a height of 40 mm 753 and the heat pulse sensor extended a rod length of 50 mm out of the ceramics. This 754 design ensures that the estimation errors for dielectric permittivity, electrical 755 conductivity, thermal conductivity and volumetric heat capacity of the porous ceramic 756 matrix are within acceptable ranges. The optimized multifunctional sensor was high in 757 accuracy, low in cost and non-destructive. More importantly, the sensor can 758 simultaneously measure soil hydrothermal properties accounting for temporal and 759 spatial variability of soil, which is of great significance for the better understating and 760 modeling of coupled water, heat and solute transport.

# 761 List of symbols

С	volumetric heat capacity	$M J m^{-3} °C^{-1}$
$C_{n-C}$	normalized ceramic volumetric heat capacity	unitless
$C_{n-S}$	normalized soil volumetric heat capacity	unitless
D	distance from the temperature measuring point to	mm

39

	the ceramic-soil boundary	
E(x, y)	electric field intensity	V/m
L	rod length	mm
$L_C$	ceramic length	mm
L <sub>max</sub>	the maximum rod length	m
$L_{min}$	the maximum rod length	m
$L_S$	length of the extended rod buried in soil	mm
p	porosity	unitless
Q	rate per unit volume of heat generation for the	$W m^{-3}$
	numerical model	
$S_H$	cross-sectional area of the heater	$m^2$
Т	temperature	°C
$V_T$	excitation voltage	V
$V_R$	reflected voltage	V
с	specific heat	$J \ kg^{-1} \ ^{\circ}C^{-1}$
$C_W$	specific heat of water	$4180 \text{ J kg}^{-1} \text{ °C}^{-1}$
d	rod diameter	mm
$f_{sa}$	sand fraction for soil solids	%
n	number of data points	unitless
q'	heat strength	$\mathbf{W} \mathbf{m}^{-1}$
qc	quartz content of the total solids content	unitless
r	rod spacing	mm
t	time	S
$t_0$	duration	S
$t_e$	travel time of electromagnetic wave	S
$v_0$	velocity of light in a vacuum	$3\times 10^8~m~s^{-1}$
w(x, y)	spatial weighting factor	$m^{-2}$
$w_C(x, y)$	weighting factors that are distributed in the ceramic	$m^{-2}$
	region	
$w_{S}(x, y)$	weighting factors that are distributed in the soil	$m^{-2}$
	region	
x	reference physical properties as preset for the	/
	medium in the simulation,	

$x_{e\!f\!f}$	estimated physical properties based on COMSOL	/
	simulation	
$x_m$	measured data in the literatures	/
$x_n$	normalized physical properties	/
$X_S$	simulated data based on COMSOL	/
β	empirical parameter	unitless
3	dielectric permittivity	unitless
E <sub>C</sub>	apparent dielectric permittivity of ceramic	unitless
$\mathcal{E}_S$	apparent dielectric permittivity of soil	unitless
$\mathcal{E}_{e\!f\!f}$	effective dielectric permittivity	unitless
$\mathcal{E}_n$	normalized dielectric permittivity	unitless
$\mathcal{E}_{n-C}$	normalized ceramic dielectric permittivity	unitless
θ	water content	$cm^3 cm^{-3}$
κ	thermal diffusivity	$m^2 s^{-1}$
λ	thermal conductivity	$W m^{-1} °C^{-1}$
$\lambda_C$	ceramic thermal conductivity	$W{\cdot}m^{-1}{\cdot}{}^{\circ}C^{-1}$
$\lambda_{dry}$	dry thermal conductivity	$\mathbf{W}{\boldsymbol{\cdot}}\mathbf{m}^{-1}{\boldsymbol{\cdot}}^{\mathbf{\circ}}\mathbf{C}^{-1}$
$\lambda_{n-C}$	normalized ceramic thermal conductivity	unitless
$\lambda_{n-S}$	normalized soil thermal conductivity	unitless
$\lambda_o$	thermal conductivity of other minerals	$W{\cdot}m^{-1}{\cdot}{}^{\circ}C^{-1}$
$\lambda_S$	soil thermal conductivity	$W{\cdot}m^{-1}{\cdot}{}^{\circ}C^{-1}$
$\lambda_q$	thermal conductivity of quartz	$7.7 \text{ W m}^{-1} \circ \text{C}^{-1}$
$\lambda_{sat}$	saturated thermal conductivity	$W{\cdot}m^{-1}{\cdot}{}^{\circ}C^{-1}$
$\lambda_{solids}$	thermal conductivity of solids	$W{\cdot}m^{-1}{\cdot}{}^{\circ}C^{-1}$
$\lambda_w$	thermal conductivity of water	$0.594 \text{ W m}^{-1} \circ \text{C}^{-1}$
		at 20 °C
ρ	wet bulk density	kg m <sup><math>-3</math></sup>
$ ho_b$	bulk density	kg m <sup><math>-3</math></sup>
$ ho_{solids}c_{solids}$	volumetric heat capacity of solids	$\rm M~J~m^{-3}~^{\circ}C^{-1}$
$ ho_w$	density of water	$1000 \text{ kg m}^{-3}$
σ	electrical conductivity	$dS m^{-1}$
$\sigma_C$	apparent electrical conductivity of ceramic	$dS m^{-1}$
$\sigma_S$	apparent electrical conductivity of soil	$dS m^{-1}$

$\sigma_{e\!f\!f}$	effective electrical conductivity	unitless
$\sigma_{n-C}$	normalized ceramic electrical conductivity	unitless
$\psi_m$	matric potential	kpa
$\nabla \Phi(x, y)$	potential gradients in homogeneous fields	V/m
$\nabla \Phi_0(x, y)$	potential gradients in heterogeneous fields	V/m

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# 763 Author contributions

HH conceptualized the study; JH and JC wrote the original paper; HH, YC,
CZ ,LJ, ZC and FZ reviewed and revised the manuscript. All authors contributed to
the discussions and provided feedback on the final version.

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# 774 Data availability statement

775 Data generated in this study is available at https://zenodo.org/records/10529525.

#### 776 **Conflicts of interest**

777 The authors declare no conflict of interest.

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