An investigation into the use of a mixture model for simulating the electrical properties of soil with varying effective saturation levels for sub-soil imaging using ECT

R R Hayes\(^1\), P A Newill\(^1\), F J W Podd\(^1\), T A York\(^1\), B D Grieve\(^1\), O Dorn\(^2\)

\(^1\)SSUIC, School of Electrical and Electronic Engineering, University of Manchester, UK
\(^2\)Inverse Problems Group, School of Mathematics, University of Manchester, UK

Email: Robert.Hayes@postgrad.manchester.ac.uk

Abstract. A new visualisation tool is being developed for seed breeders, providing on-line data for each individual plant in a screening programme. It will be used to indicate how efficiently each plant utilises the water and nutrients available in the surrounding soil. This will facilitate early detection of desirable genetic traits with the aim of increased efficiency in identification and delivery of tomorrow’s drought tolerant food crops. Visualisation takes the form of Electrical Capacitance Tomography (ECT), a non-destructive and non-intrusive imaging technique. Measurements are to be obtained for an individual plant thus allowing water and nutrient absorption levels for an individual specimen to be inferred. This paper presents the inverse problem, discusses the inherent challenges and presents the early experimental results. Two mixture models are evaluated for the prediction of electrical capacitance measurement data for varying effective soil saturation levels using a finite element model implemented in COMSOL Multiphysics. These early studies have given the research team an understanding of the technical challenges that must now be addressed to take the current research into the world of agri-science and food supply.

1. Introduction

Crops are one of the world’s major water consumers [1], as climate change leads to water scarcity there is an increase in competition for water. This severely limits irrigation and constrains food production. In the face of climate change the ability to rapidly identify new plant varieties that will be tolerant to drought, and other stresses, is going to be key to breeding the food crops of tomorrow. With large areas of Africa and South America expecting major water scarcity by 2025 [2], it is very important to develop crops that can survive in these conditions. Currently, above soil features (phenotypes) are monitored in industrial greenhouses and field trials during seed breeding programmes so as to provide an indication of which plants have the most likely preferential genetics to thrive in the future global environments [3]. These indicators of “plant vigour” are often based on loosely related features which may be straightforward to examine, such as an additional ear of corn on a maize plant, but which are labour intensive and often lacking in direct linkage to the required crop features.

A new visualisation tool is being developed for seed breeders, providing on-line data for each individual plant in a screening programme indicating how efficiently each plant utilises the water and nutrients available in the surrounding soil. It will be used as an in-field tool for early detection of
desirable genetic traits with the aim of increased efficiency in identification and delivery of tomorrow’s drought tolerant food crops.

Imaging the moisture distribution in the sub-soil environment carries a number of challenges. For in-field measurements any instrumentation must be portable, relatively low cost, internally powered and weather resistant. High resolution imaging modalities such as magnetic resonance imaging (MRI) and X-ray computed tomography (CT), while offering superior image quality, cannot be used in this capacity as the technology is costly (>£30k) and requires large high powered instrumentation (>500W). Therefore a compromise to reduce size and cost at the expense of image quality must be made. For this reason, electrical impedance imaging is an ideal candidate technology.

This modality however poses its own significant technical challenges in light of the intricacy of the medium. Electrical impedance imaging is a soft field reconstruction problem. That is to say that the regions of interaction are altered by the sample under investigation. It also suffers from being an ill-posed problem. Furthermore the medium (soil) exhibits both conductive (wet) dominating phases and dielectric (dry) dominating phases. The implication of this is the formation and breaking of conducting paths between measurement electrodes and a transition between the dominance of the real and imaginary impedance components. As a result of water loss, soil is prone to shrinking and cracking which further complicates the measurement process due to the quality of the connection at the contact points between the medium and the electrodes.

The forward solution for simulating water movement in soil measured via electrical capacitance tomography (ECT) is a complex problem and requires the consideration of several theoretical backgrounds. For this reason simulation is a valuable tool. Simulation of plant growth, root water uptake and soil water transport and the integration of these models has been an area of high activity over recent years. A number of realistic root growth models have been developed and implemented in MATLAB (including meshing functions) [4][5] and ANSI C, respectively [6]. The R-SWMS code implemented in FORTRAN 90 integrates root growth, root water uptake and soil water transport models [7]. In addition to this several commercial products such as HYDRUS 3D [8] and COMSOL Multiphysics [9] allow the simulation of soil water transport in three dimensions.

As a first step, separate ECT and hydrology models are used. However in the future these will be combined into a multiphysics model to enable joint reconstructions. Multiphysics simulation allows the relationships between different physics backgrounds to be coupled. Hence providing a means by which the required models can be combined in one software package, this is advantageous as it negates the need for interfacing two separate software packages and potentially reduces computation time. Simulation also facilitates the optimisation of sensor design by allowing a number of sensor geometries to be compared, while avoiding error introduced by measurement instrumentation as the signal-to-noise levels and power density functions can be set precisely. In addition, simulation facilitates the comparison and optimisation of image reconstruction algorithms as the ‘unknown’ permittivity distribution that is to be reconstructed can be precisely defined. Furthermore, the desire is to incorporate the simulation model into the reconstruction process so that plant water uptake can be directly estimated from the time varying moisture distribution.

COMSOL Multiphysics has been used to simulate capacitance data for a soil fluid flow experiment and will further facilitate the implementation of a multiphysics based forward solver and potentially the use of prior information in the inverse problem.

2. Background
Simulation of the electrical capacitance measurements in this application is a multiphysics problem combining, flow through a porous media to describe the movement of water through a soil column, and electrostatics for the calculation of the electrical fields resulting from the moisture distribution.
2.1. Flow in porous media

The Richards equation governs the saturated-unsaturated flow of water in non-swelling soils [10] and is given by

\[
(C + S_e S) \frac{\partial H_p}{\partial t} + \nabla \cdot \left( -K \nabla \left( H_p + D \right) \right) = Q_s
\]  

(1)

where \( C \) is specific moisture capacity (m\(^{-1}\)), \( S_e \) is the effective saturation of the soil, \( S \) is a storage coefficient (m\(^{-1}\)), \( H_p \) is the pressure head (m), \( D \) is the vertical elevation (m), \( t \) is time (d), \( K \) is the hydraulic conductivity (m/d) and \( Q_s \) is a fluid source defined by volumetric flow rate per unit volume of soil (d\(^{-1}\)).

Applying the Richards equation for a point injection with a given pressure head to a rectangular soil geometry allows the calculation of the soil water distribution at a given time. Figure 1 is an example soil water distribution obtained from the solution of the Richards equation for a rectangular soil geometry simulated using the COMSOL Multiphysics Earth Science module. The soil retention characteristics and saturated hydraulic conductivity in this example were chosen arbitrarily.

![Figure 1. 3D Simulated soil water distribution at a time, t, for a point injection.](image)

Root water uptake can be included in the Richards equation via a sink term. If a root network is considered as a series of nodes and interconnecting segments, the Doussan model can be used to calculate the water potential at each of the root nodes from a system of equations expressed in terms of the length of the interconnecting segments, the Xylem conductivity, the water potential of the surrounding soil, the radial conductivity and the surface area of the interconnecting segments [11].
2.2. Electrostatics

The forward problem in ECT is to calculate the potential distribution for a known dielectric constant and then to determine the corresponding capacitances measured at the surface. Assuming no free charge conditions, the electric scalar potential, $V$, between the electrodes mounted on the vessel satisfy Poisson's equation [12]

$$-\nabla \cdot (\epsilon_0 \epsilon_r \nabla V) = \rho$$

(2)

where $\epsilon_0$ and $\epsilon_r$ are the permittivity of free space and the dielectric constant respectively, $\rho$ is the space charge density. The electric field ($E$) and displacement field ($D$) can be obtained from the potential gradient

$$E = -\nabla V$$

(3)

$$D = \epsilon_0 \epsilon_r E$$

(4)

For the plastic surfaces of the vessel, the conditions of zero surface charge are applied at the boundary, thus

$$n \cdot D = 0$$

(5)

A finite element based implementation of this mathematical model was validated experimentally (see section 3.1).

2.3. Multiphysics Coupling

The dielectric permittivity of a partially saturated soil matrix varies as a function of water content. The implication of being able to describe this relationship mathematically is the ability to infer the water content in a soil sample via electrical measurement.

Electromagnetic techniques for inferring soil moisture content, such as time domain reflectometry (TDR) and capacitance methods [13] rely on this strong dependence of electrical signals on dielectric permittivity [14]. The permittivity can be related to soil water content using a calibration curve [15].

This consists of establishing the relationship between the signal provided by the instrumentation and the soil moisture content by using a reference method. This relationship is comprised of two subsequent relationships. Firstly the relationship between the probes output signal and the soil dielectric permittivity, which may be determined experimentally. Secondly the relationship between soil dielectric permittivity and soil water content. This may be determined using theoretical models or empirically [16].

One further interesting property of being able to mathematically model the relationship between soil moisture content and dielectric content is the potential to estimate electrical measurements (i.e. capacitance measurements) for a given soil sample based on a simulated soil moisture distribution. This provides a basis for the implementation of a multi-physics simulation.

Fluid flow and electrostatics models can be coupled via the dielectric constant, if the dielectric constant of soil can be predicted based on effective soil saturation. The dielectric constant vs. soil saturation curve may be obtained experimentally or predicted using theoretical methods.

A number of methods have been proposed to predict the dielectric constant of water saturated rocks and soils at varied soil saturation levels. Two of the more popular theoretical methods are the Topp model [17] and the Complex Refractive Index Method (CRIM) [18]. These methods have been tested extensively [19][20] and are commonly used in the calibration of dielectric soil moisture probes [14].
The popular empirical model known as the Topp model was developed by Topp et al by compiling data for many soils under varying moisture conditions [21]. This model is given by the third-order polynomial equation

$$\varepsilon = 3.03 + 9.3\theta + 146\theta^2 - 76.7\theta^3$$

(6)

where $\varepsilon$ denotes the effective dielectric constant of the soil mixture and $\theta$ denotes the water content. Extensive testing has shown the Topp model to be reasonably accurate for many soils [22]. However, its validity has not been demonstrated over a full range of possible water contents and porosities [23].

The complex refractive index method (CRIM) involves using simple mixing laws to calculate the dielectric constant of a material ($\varepsilon_T$) given the dielectric constant ($\varepsilon_i$) and the volume fraction ($V_i$) as given by

$$\sqrt{\varepsilon_T} = \sum_i V_i \sqrt{\varepsilon_i}$$

(7)

This can be expanded for the case of a soil sample at a given level of water saturation ($\theta$), where $\theta$ is the volume fraction of the pore space that is filled with water, the remainder being filled with air [24]. The system is composed of soil ($\varepsilon_s$), water ($\varepsilon_w$) and air ($\varepsilon_A$). Porosity is given by $\phi$ and the dielectric constant for a given soil saturation level is expressed as

$$\sqrt{\varepsilon_T} = (1 - \phi) \sqrt{\varepsilon_s} + \theta \phi \sqrt{\varepsilon_w} + (1 - \theta) \phi \sqrt{\varepsilon_A}$$

(8)

Assuming that the soil and air components have negligible conductivity, the dielectric constants of both soil and air can be assumed to be entirely real[24][25].

An obvious limitation of both models is that they assume localised homogeneity and complete mixing. They also do not take into account electro-chemical interactions amongst the constituent components [24].

This paper will discuss the validity of the FEM model and compare simulated capacitance data, based on the dielectric permittivity predicted by the Topp and CRIM models, with measured capacitance data (see section 3.2).
3. Experimental Procedure and Results

3.1. Validation of the FEM through observing the effect of water fill level

In order to validate an electrostatic simulation implemented in COMSOL Multiphysics, the capacitance of a rectangular vessel as described in figure 2 was measured for varying water fill levels. The vessel walls were manufactured to include two parallel plate electrodes of dimension 130mm x 85mm as shown in figure 3. These electrodes were insulated from the medium using a solder mask layer of 75μm thickness. Measurements were carried out using a Hewlett Packard 4192A Impedance analyser.

The dielectric constant of the solder mask layer was set to 3.56 (as defined by the manufacturer) in the FEM. Simulations were then carried out for fill levels ranging from 0mm (100% air) to 120mm (100% water) in 10mm steps. The dielectric constant of air was taken as 1.00059 [26] and the dielectric constant of water was taken as 79 at 20 degrees Celsius [27][28].

![Figure 2. Schematic diagram of the rectangular vessel. Left: Front view, Right: Top view.](image)

![Figure 3. Left: Vessel wall showing electrode Right: Constructed measurement vessel](image)
A comparison between measured and simulated data is shown in figure 4. The point at which both measurement sets cease to increase linearly is the point at which the water fill level exceeds the height of the electrode. Beyond this level, the change is in the fringing field only and variations are of ~11pF corresponding to approximately 3% of the total measured capacitance. The maximum error between simulation and measurement is 43.64% corresponding to an error of 5.26 pF. This error occurs when the vessel is empty, i.e. filled with air. This point is the lowest measured capacitance, hence the most sensitive to measurement error. The average error is 8.88%. Possible sources of error include experimental error and the absence of temperature data in order to account for the temperature dependency of the dielectric constant of water. Analysis of the potential sources of error is presented in section 3.3.

Figure 4. Plot of capacitance vs. fill level for measured and simulated capacitance data.

Figure 5 shows the simulated electric fields for a half filled vessel. Note the electric field is highest in the region of higher dielectric constant (i.e. the water) as represented by the largest arrows. The smaller arrows represent the weaker electric field in the air filled region.
3.2. Varying soil saturation
To determine the validity of the Topp and CRIM models, the HP impedance analyser was also used to measure the capacitance of the vessel when filled with soil of varying levels of saturation. The dielectric constant of the soil matrix was predicted for the corresponding saturation levels using both the Topp and CRIM models. For the CRIM model porosity was taken as 0.54. This value was calculated from data provided by a soil analysis service offered by Forest Research Surrey using the following

\[ \phi = 1 - \frac{\rho_{\text{bulk}}}{\rho_{\text{particle}}} \]  \hspace{1cm} (9)

where \( \phi \) is the porosity, \( \rho_{\text{bulk}} \) is the bulk density, defined as the average density of dry soil. \( \rho_{\text{particle}} \) is the particle density, defined as the density of the particles that the soil consists of. It is equal to the dry density of the solid material comprising the soil matrix i.e. the mass of air is negligible [29]. The particle density of a soil may be estimated using the weighted average of the solid components [29] and is given by

\[ \rho_{\text{particle}} = \rho_m X_m + \rho_{om} X_{om} \]  \hspace{1cm} (10)

where \( \rho_{\text{particle}} \) is total soil density, \( \rho_m \) and \( \rho_{om} \) are the mineral fraction density and organic matter fraction density respectively, \( X_m \) and \( X_{om} \) are the mineral volume fraction and the organic matter volume fraction respectively. The porosity value of 0.54 is consistent with values for silty soils [30].
The predicted dielectric constants from the Topp and CRIM models were substituted into the FEM and the respective capacitance measurements were calculated by simulation.

As the soil water content was increased, the capacitance measurements had two distinct regions of linearity, as can be seen in figure 6. Any non-linearity is likely to be caused by inconsistencies in the level of compaction of soil and/or any bowing of the vessel wall between subsequent measurements.

![Figure 6](image)

**Figure 6.** Measured and simulated capacitance measurements vs. soil saturation level.

Beyond a saturation level of ~20% there is a sudden increase in the slope. This discrepancy to the mathematical model is believed to be the result of resistive coupling on the reading from the HP impedance analyser for conductivities greater than 0.48 mS. Distilled water was used. However the mineral content of the soil increased the conductivity of the water from 0 mS to 0.75 mS. This hypothesis was investigated by repeating the procedure using a non-conductive liquid (Rapeseed oil) to saturate the soil. It is assumed that the ions present in the soil are not oil soluble and do not increase the conductivity of the oil. An equivalent experiment using “washed” sand and distilled water was also carried out.

The CRIM equation was used to predict the dielectric constant of the soil/sand matrix for varying saturation levels and substituted into the FEM to simulate the expected capacitance measurement data. This simulated data was compared with measured data. In this case, the dielectric constant of rapeseed oil was taken as 3.1 [31]. The Topp model was not considered in these experiments as it is formulated for a soil-water matrix and cannot be modified to describe other components.

As can be seen in figures 7 and 8, the change of slope is no longer present. This suggests that the hypothesis of instrumentation limitations for high conductivities appears valid. Any non-linearity in the measured data is likely due to variations in the level of compaction between subsequent measurements. Predictions based on the CRIM model had an average error of 3.77% and 5.25% for the soil-oil and sand-water experiments respectively as compared to measured data.
Figure 7. Measured and simulated capacitance measurements vs. level of soil saturation using rapeseed oil.

Figure 8. Measured and simulated capacitance measurements vs. level of sand saturation using distilled water.
It is thought that at lower measurement frequencies the effects of soil type and soil conductivity are prevalent. The result is a requirement for higher excitation frequencies this is due to decreased conductive losses at higher frequencies hence reducing the effect of soil conductivity [32]. At present the measurement instrument is limited to 1MHz. The result of using a higher frequency is a simplification of the calibration process. In many cases a single calibration curve may be used for numerous soil types [33]. The literature suggests that using suitable calibration curves capacitance measurements can provide reliable results over the full typical range of saturation levels (0-60%) [13][34]. Typically soil dielectric measurement instruments operate in the 10-200 MHz region [13].

3.3. Investigating the source of error

In order to determine the sensitivity of measurement data with respect to temperature, the variability of the dielectric constant of water vs. temperature was investigated. The variation of dielectric constant of water with respect to temperature was modelled using the polynomial equation [35]

\[
\varepsilon_w = 5321T^{-1} + 233.76 - 0.9297T + 0.1417 \times 10^{-2}T^2 - 0.8292 \times 10^{-6}T^3
\]  

(11)

where \(\varepsilon_w\) is the dielectric constant of water and \(T\) is the temperature in Kelvin.

The modelled dielectric constant of water for the temperature range of 0 to 100 degrees Celsius is shown in figure 9. The standard parallel plate capacitor equation was then used to calculate the capacitance for the vessel fully filled with distilled water. The thickness and dielectric constant of the dielectric layer is known. The dielectric constant of water was taken as 79 at 20 degrees Celsius [35]. These values were taken as a reference. To determine the extent to which the measurements were sensitive to temperature changes of water, the dielectric constant of water was varied until the resulting expected capacitance changed by \(\sim 10\%\) of the reference. This corresponds to a change of 12.6% in the value of the dielectric constant of water which is equivalent to a temperature rise of approximately 25-30 degrees Celsius. This results in a temperature of approx 50 degree Celsius. It is unlikely that such an error in temperature measurement occurred. Figure 10 shows the change in capacitance calculated for the temperature varied dielectric constant of water.
Figure 9. Variation of the dielectric constant of water with respect to temperature.

Figure 10. Error in predicted capacitance vs. temperature induced drift in dielectric constant of water for determining the extent to which the temperature dependence of the dielectric constant of water contributes to measurement error.
4. Conclusions

4.1. Initial findings
Experiments have shown that the simulation is able to predict changes in capacitance due to varying levels of soil saturation based on two methods for predicting the dielectric constant of varying soil water saturation levels.

The electrostatic model has been shown to exhibit an average error of 8.88% for varying water fill levels in comparison to measured data. Predictions generated using both the Topp and CRIM models were compared to measured data for varying soil saturation levels. It has been noted that beyond 20% soil saturation, there are difficulties in measuring the capacitance of the wetted soil. This has been attributed to the limitations of the measurement instrumentation for highly conductive media.

The CRIM model was evaluated for two further matrices in addition to water wet soil. This was not possible with the Topp model as this relation is only valid for a matrix of water wet soil. Predictions based on the CRIM model had an average error of between 3.77% and 5.25% for the soil-oil and sand-water experiments respectively compared to measured data. As a result, the CRIM model will be implemented in COMSOL multiphysics to couple the electrostatic simulation to the soil transport simulation to allow for multiphysics simulations.

Experiments have shown that the temperature dependency of the dielectric constant of water will not contribute substantial error over the normal operating temperature range of the instrument. However temperature correction may be easily integrated using a simple mathematical model [35].

Ultimately, for further evaluation of the simulation it is felt that a higher frequency range will improve capacitance measurement capabilities for water-wet soils. Typically soil dielectric measurement instruments operate in the 10-200 MHz region [13] however the current instrumentation is limited to 1 MHz. It is anticipated that a measurement range up to 75 MHz will be sufficient [33].

4.2. Future work
Some time must be spent to further understand the limitations of the measurement instrument. Ideally a calibration curve may be generated using complex impedance measurements, allowing the correction of measurement data and hence extending the measurement range of the instrument.

Further work will be carried out to greater parameterise the soil samples. In doing so any uncertainty regarding the current porosity value will be minimised, this will allow a better comparison between the Topp and CRIM models.

The current measurement vessel will be replaced with one allowing the spatial moisture distribution to be mapped, i.e. a vessel with a larger number of independent electrodes.

Fluid flow in a porous media and electrostatics models have been implemented in isolation, this paper focused only on the latter. These models will be coupled through the dielectric constant vs. soil saturation curve as predicted by a mixture model. This will allow the simulation of electric fields due to varying soil water distributions hence facilitating the implementation of a multiphysics based forward solver in COMSOL multiphysics. The forward solver will be optimised for typical tomographic vessel geometries and will allow the generation of calibration curves in order to correct for measurement error. Ultimately a fully integrated electrostatics model based on the fluid flow as predicted by the Richards equation will be developed.

In the long term, the soil retention curves will be obtained experimentally and the resulting parameterisation substituted into the Richards equation solver in COMSOL Multiphysics. Root growth models and root water uptake models will be integrated into the multiphysics models. The final, fully integrated model will be used in the reconstruction of ECT images and enable prior information in the inverse problem.
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