



Evaluation of TrueCell program for estimating point capillary pressure – saturation parameters for Flint sand



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ABSTRACT

The purpose of this paper is to compare inverse estimates of point capillary pressure–effective saturation, $S_e(\psi)$, parameters and functions with independently measured $S_e(\psi)$ parameters and functions. Average capillary pressure–effective saturation functions, $\langle S_e \rangle(\psi)$, were measured for Flint sand using a hanging water column setup and 9 packed columns, with heights varying between 4.3 cm and 55.0 cm. TrueCell, a Fortran program, was employed to inversely estimate point $S_e(\psi)$ parameters and functions from the $\langle S_e \rangle(\psi)$ data sets. The TrueCell estimates were then compared with point $S_e(\psi)$ parameters and functions determined by neutron radiographic imaging of a single hanging water column setup. One sample t-tests indicated that there were no significant differences (at $p < 0.05$) between the mean values of the inversely estimated point parameters and the corresponding neutron imaging values. However, the individual TrueCell predictions produced variable results compared to the measured point parameter set. Relatively few parameter estimates fell within the 95% confidence intervals of the neutron imaging estimates, and some deviations were quite large. These deviations were related to subtle variations in column packing, rather than differences in column height. Although this study has produced support for inverse modeling with TrueCell, it is important to note that individual predictions of $S_e(\psi)$ parameters and functions were often at odds with the independent measurements. Thus, TrueCell should be used with caution. In future studies of a similar nature, it would be desirable to independently determine point parameters and functions on multiple columns, rather than on a single column as was done here. Additionally, future research might want to examine the relationship between variations among individual parameters within a parameter set and the resulting predicted function.

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1. Introduction

The capillary pressure–saturation function is a key hydraulic property used to characterize water retention in the vadose zone and to facilitate the prediction of relative permeability. Parameters describing this function are used as model inputs to numerically simulate a variety of critical hydrologic issues related to the environment (e.g., permafrost thawing due to climate change, fate and transport of contaminants in the vadose zone) and energy resources (e.g., oil and gas recovery, geologic carbon sequestration in confined brine aquifers).

The capillary pressure–saturation function is frequently determined experimentally in the laboratory by measuring outflow from a sample of finite height as it is subjected to a series of step changes in capillary pressure using a hanging water column, pressure cell, or centrifuge. Changes in average saturation within the sample are determined from the outflow measurements. Parameters for input into numerical models are then obtained by fitting a mathematical expression, such as the Brooks and Corey (1964) (BC) equation or the van Genuchten (1980) equation, to the average saturation versus capillary pressure data pairs using the method of least squares. However, the resulting parameter estimates depend upon the sample dimensions and experimental setup (Cheng et al., 2013).

If the distribution of liquids within the sample is unknown, then the capillary pressure–saturation function at any physical point in the sample, $S(\psi)$, is also unknown. As a result, hanging water column, pressure cell, and centrifuge experiments produce an average capillary pressure–saturation function for the sample, $\langle S \rangle(\psi)$, rather than the point, $S(\psi)$, function. Parameters describing the $\langle S \rangle(\psi)$ depend upon the sample/

Abbreviations: RMSE, Root mean square error; BC, Brooks and Corey; TDR, Time-domain reflectometry.

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cell height over which the averaging has been measured. Average $\langle S \rangle(\psi)$ functions can differ significantly from point $S(\psi)$ functions (Cropper et al., 2011).

Liu and Dane (1995a) derived analytical expressions, based on height-averaging, that relate the point, $S(\psi)$, function to the average function, $\langle S \rangle(\psi)$:

$$\psi = \langle \psi \rangle + z_n \frac{\rho_n}{\rho_w} - z_w + \left(1 - \frac{\rho_n}{\rho_w}\right) z \quad (1a)$$

$$\langle S \rangle = \frac{1}{z_c} \int_0^{z_c} S(\psi) dz \quad (1b)$$

where $\langle \psi \rangle$ is the average capillary pressure head, $\langle S \rangle$ is the height averaged relative saturation, ψ is the point capillary pressure head, S is the point relative saturation (location dependent), z_n and z_w are the heights where the pressures of the non-wetting (i.e. air) and wetting (i.e. water) fluids are measured respectively, z is the height at a point, z_c is the cell height, and ρ_n and ρ_w are the densities of the non-wetting and wetting fluids respectively. Eq. (1a) and (1b) allows for the inverse determination of point functions from average functions obtained using experimental methods such as the hanging water column, pressure cell, or centrifuge.

Point water retention functions are more likely to have an obvious air entry value than average functions (Sakaki and Illangasekare, 2007; Cheng et al., 2013). Thus, parameterization using the BC equation, which has a pronounced break in slope at this value, is preferred over fitting the van Genuchten (1980) equation which is a continuous function. Liu and Dane (1995b) used Eq. (1a) and (1b) to inversely estimate point parameters for the BC equation from average pressure cell retention data. Jalbert et al. (1999) introduced a FORTRAN-based computer program (TrueCell) that automates this process. The TrueCell program is recommended for use in the standard reference on physical methods of soil analysis (Dane and Hopmans, 2002). However, Liu and Dane (1995a, 1995b) and Jalbert et al. (1999) never validated the TrueCell approach against actual measurements of point capillary pressure–saturation functions.

In contrast to methods based on measuring outflow, time domain reflectometry (TDR) and various digital imaging technologies allow the distribution of liquids to be measured within a sample as it is subjected to step changes in capillary pressure. Sakaki and Illangasekare (2007) measured point $S(\psi)$ functions using TDR probes installed at the mid-point of sample height in nine columns of sandy materials. Imaging technologies such as gamma beam attenuation (Dane et al., 1992), magnetic resonance imaging (MRI) (Chen and Balcom, 2005), neutron radiography (Kang et al., 2014), and X-ray computed tomography (CT) (Bayer et al., 2004) have also been successfully employed to determine point capillary pressure–saturation curves for various porous media.

Despite the availability of appropriate measurement techniques, we are only aware of two previous studies that have validated the performance of the TrueCell program against independent point water retention data. Sakaki and Illangasekare (2007) and Kang et al. (2014) compared point BC parameters extracted from average saturation data using the TrueCell program with those obtained from actual point measurements of $S(\psi)$. Both studies found reasonable agreement between the measured point BC parameters and the estimates from TrueCell. However, the samples investigated within each study, were all the same height. Given the inclusion of TrueCell in the standard text on physical methods of soil analysis, a more robust validation, with samples of varying heights, is warranted.

The objective of this paper is to test the hypothesis that TrueCell can be employed to predict point BC parameters based on measured average capillary pressure–saturation data collected over a wide range of sample heights. To facilitate the drainage process and reduce other sources of experimental variability we employ a single homogenous

porous medium: Flint sand. Our comparison is achieved through the following steps:

- (i) Measure average water retention in Flint sand columns of various heights using the hanging water column method;
- (ii) Use TrueCell to extract point BC equation parameters from the observed average retention data;
- (iii) Fit the BC equation to point capillary pressure–saturation functions measured on Flint sand by Kang et al. (2014) using neutron radiography;
- (iv) Compare point BC parameters obtained from the point and average data sets and their predicted capillary pressure–saturation functions.

2. Materials and methods

2.1. Flint sand

Flint sand (Flint #13, U.S. Silica Company, Berkeley Springs, WV) was selected as the material for this study. It is a relatively coarse homogeneous porous medium, facilitating relatively short pressure equilibrium times over the range of column heights studied. Sand grain diameters for this material range from 0.11 to 0.60 mm with a median grain diameter of 0.56 mm. It is mainly composed of quartz (99.8%), has a particle density of $2.65 \times 10^3 \text{ kg m}^{-3}$, and a saturated hydraulic conductivity of $1.66 \pm 0.32 \times 10^{-4} \text{ m s}^{-1}$ (U.S. Silica Company, 2009).

2.2. Point function data and parameterization

Kang et al. (2014) employed neutron radiography combined with a hanging water column setup and quasi-equilibrium drainage technique to characterize the point drainage behavior of a 5.6 cm tall column of Flint sand. The method is based on measuring the transmitted intensity of neutrons through a sample. Neutrons are attenuated differently by water and mineral solids. Through calibration the spatial distribution of water is obtained by mapping the attenuation of neutrons transmitted through the sample. The capillary pressure–saturation behavior at any point within the sample can then be determined by observing changes in the volumetric water content (θ) during quasi-equilibrium drainage increments.

The Kang et al. (2014) data set comprised 1080 paired observations of volumetric water content and capillary pressure head, with capillary pressure heads ranging between 2.66 cm and 51.73 cm. The data pairs were measured at different locations (corresponding to the intersections of an 8 by 15 grid) within the column, and were originally analyzed as 120 separate point capillary pressure–saturation curves. In the present study, these data were converted to effective saturation versus capillary pressure head data pairs, and were analyzed as a single point function for the entire column. Effective saturation, $S_e = (\theta - \theta_r) / (\theta_s - \theta_r)$, was calculated using the observed saturated (θ_s) and residual (θ_r) volumetric water contents. The volumetric water content at saturation ($0.391 \text{ m}^3 \text{ m}^{-3}$) was determined by averaging the eight (maximum) volumetric water contents measured at the minimum imposed capillary pressure head (2.66 cm). The residual volumetric water content ($0.018 \text{ m}^3 \text{ m}^{-3}$) was determined by averaging the eight (minimum) volumetric water contents measured at the maximum imposed capillary pressure head (51.73 cm).

The resulting effective saturation–capillary pressure data set was parameterized with the BC equation by fitting all 1080 data pairs to produce a composite point water retention function for Flint sand. The BC equation was fitted in the following form:

$$S_e(\psi) = \left(\frac{\psi_a}{\psi}\right)^\lambda \{\psi > \psi_a\} \quad (2a)$$

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