Challenges in Matching Permeability Observed in Macroporous Soil with Lattice Boltzmann and Image Analysis Methods Using Segmented Pore Structures.

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**ABSTRACT**

Advances in experimental technique and computing technology have made it possible to observe and characterize fluid dynamics at the pore scale. Two modeling approaches are tested. Lattice Boltzmann methods (LB) have been shown to represent complex geometries and return macroscopic observations from microscopic fluid vectors. However, computational fluid dynamics such as LB are limited by computational resources and time. The Kozeny-Carman equation has the distinct advantage of being much less computationally demanding. Four silt loam macropore soil columns were modeled using both LB and KC equations. x-ray computed tomography was used to capture three-dimensional digital imagery of each soil column. Each soil column was later split into eight even sections, and each section was binarized with six separate algorithms to observe variability in the image preparation process. Permeability of each segmented section was modeled with both KC and LB methods. Apparent failure of both modeling methods is observed with this data set. Estimated permeability from both methods and all segmentation algorithms returned permeability values ranging from -2 orders of magnitude less than to 4 orders of magnitude larger than laboratory observations. Variation of up to 4 orders-of-magnitude in modeled permeability exist as a result of chosen segmentation standard. Inability of the CT methods to capture and represent organic materials also contributed to higher model permeability. Comparison of LB and KC model results yields a relationship of (r2 = 0.76) which is stronger than the best correlations with observed permeability.

**1 Introduction**

The quantification of permeability, an intrinsic property of porous media, has widespread industrial and environmental applications such as oil and gas production (*Stone 1973*), water treatment and membrane design (*Pendergast 2011*), contaminant transport (*Mulligan 2001, Berkowitz 2002*), remediation practices (*Waybrant 1998*), and aquifer characterization. Permeability of soils and rock is typically measured in laboratory with fluids (*Fetter 2001*) or gases (*Ferreira 2010*). The measurement of permeability in macroporous soils or rock poses unique challenges because standard petrophysical methods such as air permeability, constant head and falling head methods have limitations on the maximum flow rates they can handle (*Sukop 2013*).With these limitations in mind, it is useful to evaluate alternative methods for determining permeability in macro-porous media. One such approach is to derive permeability through deterministic computational fluid dynamics (CFD) methods that simulate the 3D pore-scale level flow in pore structures obtained from computer tomography (CT) scans of (macro)porous media (*Spanne 1994, Hilpert 2011, Sukop 2013*). In effect, laboratory measurements are replaced by simulations and the permeability is recovered from simulated sample-scale flow rates and imposed boundary conditions, CFD methods are computationally expensive (often taking hours to days of computation time) and a case can be made to use semi-empirical methods, such as the Kozeny-Carman (KC) equation (Carman 1937, 1939), which typically require estimates of porosity and tortuosity and do not need pore-scale level simulations of fluid flow. The input required for the KC equation can be derived from image analysis of thin sections (*Schaap 2001, Oren and Bakke 2003*) or from the same CT scans used for CFD computations.

The success of CFD or KC methods to estimate permeability in macroporous media strongly depends on whether CT scans of porous media and subsequent image processing can accurately represent the original porous medium. CT scans have been instrumental in gaining new insight about pore connectivity (*Vogel 2000*), spatial correlation and tortuosity (*Coles et al. 1998*), volumetric water content (*Hopmans et al. 1992*), contaminant transport (*Clausnitzer 2000*), colloidal transport (*Gaillard et al. 2007*), and fluid flow using lattice Boltzmann model (*Chen 1998*). There are a number of CT systems available to the researcher, each differing in x-ray source and intensity, detector geometry, permissible sample size and resolution scale (*Ketchum 2001, Wildenschild 2002*). These include synchrotron systems, which provide high intensity monochromatic x-rays and can resolve to the micron scale. While these methods permit scans within minutes, they typically permit only mm to cm-scale samples. Conversely, medical CT systems permit scans of much larger objects and are designed for soft tissue imaging, but typically have relatively course (mm scale) resolution. Industrial (benchtop) systems appear to be the most suitable for the study of macro-porous soils by utilizing a broad spectrum x-ray source and by permitting relatively large samples with a sub-mm resolution.

The gray-scale volumes acquired by CT methods typically have ambiguity whether a particular voxel (volume element) belongs to a particular phase. This uncertainty is in part due to sources of noise and in part because of the partial volume effect that makes it impossible to resolve pores smaller than the resolution used. Quantitative analyses on CT volumes often require a segmentation step that classifies individual voxels into distinct phases (gas, liquid, solid). Segmentation schemes are susceptible to image artifacts present in the CT collection and reconstruction process (*Ketchum 2001*). There are many segmentation algorithms to choose from. Indeed, over one-hundred different segmentation algorithms have been identified in the literature, each of which can be classified by general methodology (*Iassonov 2009*). Each method can return different representations of pore boundaries and has the potential of yielding different pore structures and consequently different permeabilities. An important question is, therefore: which segmentation methods are suitable for accurately resolving macroporosity? In addition we can ask how the choice of segmentation algorithm affects the permeability derived with CFD or KC methods. Finally, since we are primarily interested in sample-scale permeability, it is useful to evaluate whether a pore-scale CFD method has advantages over a much simpler KC approach.

The formal objective of this study was two-fold. Firstly, we evaluated six representative segmentation algorithms that would be suitable for largely automated operation and minimization of operator bias (Iassonov, 2009). We evaluated these six segmentations according to total porosity, hydraulic radius, estimated tortuosity and Euler number, which is a metric of pore-space connectivity. The hypothesis was that more-sophisticated segmentation algorithms would be better at delivering segmented pore volumes that were suitable for representing laboratory observed permeability in macro-porous soil. Secondly, we estimated the permeability using CFD (using a lattice Boltzmann, LB, method) and with the Kozeny Carman equation using input derived from image analysis on the segmented volumes. Here, it was hypothesized that the LB would be better in estimating permeability than a KC-based method for the simple reason that the LB simulated the actual pore-scale flow process in the 3D volume, whereas the KC method did not consider the flow process itself. The third objective of this paper is to discuss the relative value of each method in the context of estimating macropore permeability.

**2 Methods**

*2.1 Field and Laboratory Methods*

Cylindrical soil columns of 7.5 cm diameter and 20 cm height were collected from a livestock grazing site on a floodplain in Franklin County, Pennsylvania, USA. The soils were collected from the A horizon of a fine-silty, mixed, mesic, Aeric Fragiaquults (soil survey staff, 1999). Site soil texture was noted as 28% sand, 46% silt, and 26% clay with 3.3% organic matter present at the site, and bulk density was recorded as 1.43 g cm-3 (*Martinez et al. 2010*). Nine columns were collected in total, but available time limited CT scans to columns 3, 7, 8 and 9 which are the therefore the primary focus of this study.

Saturated hydraulic conductivity measurements were performed *after* CT scanning (which is described in the next section). Soil columns were saturated and placed on a perforated disk inside of a funnel. Water head of 25 mm was kept constant on soil surface, and outflow was measured for each soil column over a 10 minute period with 1 minute sample intervals. Constant water level was maintained manually with an accuracy of 2 mm in this study. This procedure was repeated 3 times and linear parts of the cumulative outflow curves were used to calculate the saturated hydraulic conductivity.  Measurements were made for the full soil column (16.28cm), followed by cutting and measuring for eight, approximately 2-cm sections of each column. was converted to permeability following the relationship:

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|  |  | [1] |

where dynamic viscosity and fluid density where assumed to be at standard temperature and pressure during laboratory procedures. The harmonic mean permeability of the eight, 2.035cm sections was compared to the full permeability by calculating (*Prakash 2013*):

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where *i* is the section number with *n*=8, is the section length, and is the permeability.

Table 1 shows the comparison between for the harmonic mean of the 2-cm sections and the calculated permeability value for the intact column. This metric provides insight into possible damage to the pore structure during the cutting process. The harmonic mean for columns 3 column 9 were larger than the permeability of the intact soil columns (Table 1), which suggests that isolated or non-percolating pores which were present in the intact columns are able to percolate in the eighth sized sections after cutting. Laboratory results from column 7 and column 8 showed slightly less than a 1:1 ratio between harmonic mean permeability and the permeability of the intact soil columns (Table 1). A lower harmonic mean permeability suggests that during the cutting process, some previously undisturbed pores may have been deformed or even destroyed. Smearing and destruction of the original pore structure during cutting would subsequently reduce the overall permeability of the cut sections. Since CT scanning was performed on the intact columns before the permeability measurements and cutting, any smearing that was not imaged and caused a potential for disagreement between observed and LB and KC-derived permeabilities. However, the cutting process itself can be replicated on the imaged cores and does not cause a deviation in observed and derived permeabilities.

Although no soil water retention curves were measured for columns 3, 7, 8, and 9, the CT imaged soil columns observed in this study, a soil water retention curve was collected for Column 1 (Figure 1). This soil column was collected from the same floodplain grazing site and is considered representative of the four macropore soil columns studied in this paper. A pore size distribution was calculated for Column 01 using the relationship

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|  |  | [3] |

where describes the matric potential component of the soil water characteristic at the corresponding pore diameter (*Schjønning* *2009*). The retention data collected and the estimated pore-size distribution appear in Figure 1.

*2.2 CT Procedures and Column Cropping*

A HYTEC Flat Panel Amorphous Silicon High-Resolution Computed Tomography (FLASHCT) system at Washington State University was used to image the dry cores at 380 keV and 1.7mA current and a resolution of 110 μm/voxel. Copper filters were used between the x-ray source and the soil columns to pre-harden the beam. The resulting CT radiographs were reconstructed to volumes of 820 x 820 x 1480 voxels (*Martinez et al. 2010*) which were cropped to 680 x 680 x 1480 voxels to remove unused negative space. Separation of the soil samples from their polycarbonate cylinders as a result of storage and transport was visually observed prior to CT scanning (*Martinez 2010*) but not present during the permeability measurements. After segmentation (discussed next) we found that the outer 15 voxels of most the sample sections had artificial and *percolating* porosity that would seriously impair a comparison between observed and derived permeabilities. For this reason, we removed an outer ring of 15 voxels from the imaged volumes. For the sake of brevity we do not show details about this additional cropping step, but we do note that the digital volumes used for the LB and KC analyses were somewhat narrower than the samples used for permeability measurements (6.82 and 7.15cm in diameter, respectively). Results presented in this study became substantially worse when this procedure was not carried out (not shown).

*2.3 Segmentation Methods*

Standardization of segmentation methods is critical to the field of pore scale modeling (*Marcelino 2007*). For this reason each segmentation method chosen was selected for the ability of the algorithm to be automated which, in principle, would minimize operator bias. Intensity variations due to beam hardening artifacts were corrected before segmentation with the Intensity Correction Procedure (ICP) described in *Iassonov 2010*. In addition to ICP, a radially weighted local regression model was applied to reduce residual beam hardening effects on each of the columns (not shown). Finally, median filtering was applied in an attempt to fully remove noise and image artifacts (*Astola 1990*).

Initially six algorithms that represented a wide spectrum of algorithms were chosen and for the sake of brevity we refer to *Iassonov 2009* for a detailed description and classification. The algorithms include four “global” methods (i.e. segmentation parameters are set for the volume as a whole): thresholding (*Rosin 2001*), clustering (*Otsu 1979*), Entropy based methods (*Brink 1992*; *Yen 1995*). The two “local” methods use information in the neighborhood of a voxel to make a classification and include indicator kriging (IK, *Oh and Lindquist 1999*) and a Markov Random Field method (KMMRF, *Kulkarni 2012*). An example of an original CT volume and the results of each segmentation is shown in Figure2 for section 2 of Column 3.

*2.3 Image analysis methods*

After segmentation, the resulting 3D pore structures are immediately ready for the LB computations. However, for the KC method additional image analysis needs to be performed to derive porosity, and hydraulic radius. Porosity was calculated using the standard volume based definition of porosity

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|  |  | [4] |

where and define the number of image voxels associated with each segmented phase.

Hydraulic radius is a commonly used hydrological metric that describes the ratio of the cross sectional area of a channel divided by the wetted perimeter of that channel. This description of provides a two-dimensional relationship. This relationship is modified to represent a three dimensional system by assuming the wetted perimeter extends to all pore-solid contacts within a saturated system using the equation:

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|  |  | [5] |

where refers to the volume of pore voxels and is the total area of pore to solid contacts. Theoretically, is equivalent to exactly half of the radius for a cylindrical pore.

For the interpretation of the segmentation, LB, and KC results it is useful to quantify soil pore structure by the Specific Euler number:

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|  |  | [6] |

where is the number of isolated pore voxels, is the number of connections between pore voxels, describes the number of voxels in completely enclosed cavities, and is the total number of voxels in the volume (*Vogel 2000, Doube 2010*). The specific Euler number calculation shows that as the hydraulic connectivity of a sample increases will become more negative.

*2.4 CFD (Lattice Boltzmann) Estimates*

CFD methods have become attractive to analyze 3D pore volumes derived from CT scaling and image segmentation. The lattice Boltzmann Method (LB) is one such CFD system, which is applied primarily for its relative ease of implementation on computer clusters and its ability to simulate pore-scale fluid flow in complex geometries. Although computationally intensive lattice Boltzmann methods have been shown to fully recover the Navier-Stokes equation (*Qian 1992; Benzi et al. 1992*) and has been used to simulate the permeability of saturated porous media (*Ferreol 1994, Martys 1996, Keehm 2004, Zhang 2005, Carmago 2011, Hilpert 2011, Sukop 2013*), gain insights into multiphase and multiple component flow (*Shan 1993, Martys 1996, Schaap 2007*). In addition, LB methods have been used to simulate heat transport (*He et al 1998*) and represent enhanced colloidal transport (*Laad 2001*).

Lattice Boltzmann computational fluid dynamics is a refinement of lattice gas automata (*Frish et al. 1986*). The discretization processes and application of simple bounce back rules enables the representation of complex geological structures. Application of either body force or pressure boundary conditions (*Zou and He 1997*) drives flow within the system. A single relaxation time, three dimensional, nineteen fluid node (D3Q19) lattice Boltzmann fluid CFD was selected for this study and we refer to Chen and Doolen 1996 and Sukop 2007 for details on the numerical approach. Pressure boundary conditions according to *Zou and He* (*1997*)were applied to cause flow in the LB simulations. LB simulations were performed under saturated conditions for each of the soil sections. Each modeled section has a domain size of 185 x 622 x 622 voxels, of which 185x620x620 was actual sample volume. Image resolution was 110 . Models were run for up to 400,000 iterations to reach steady state conditions which were assumed when the change vertical flow rate reached levels of less than 10-7 in LB units.

LB simulations return fluid densities and velocities at the voxel scale in effectively non-dimensional lattice units. Dimensionalization of lattice Boltzmann fluid domains into physical quantities is covered in detail by *Hilpert* (*2011*) *and Sukop* (*2013*). Dimensionalization of LB results in this study was accomplished through Darcy’s law, written in permeability form:

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Where *q* is the flow rate pressure gradient is the domain length in voxels and. Lattice dynamic viscosity must be calculated from shear viscosity to return a non-dimensional lattice permeability. For both LB and KC models, dimensionless permeability values can be scaled to physical units using the image resolution of the porous media used for CFD simulation.

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Hydraulic tortuosity can be directly calculated using the primary macroscopic fluid velocity vectors recovered through the momentum density calculation outlined in the equation of state.

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*2.5 Kozeny-Carman Estimates*

Semi-empirical models to estimate the permeability of porous media such as the well-known Kozeny-Carman relationship (KC, *Carman 1937, 1939*) are of value because they do not need to compute the actual flow processes at the pore-scale and are therefore less computationally demanding. Unlike hydraulic conductivity, permeability is a function of only the pore structure, and for straight pores can be described by Torsional rigidity theory as:

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|  |  | [10] |

where describes the pore radius and is a shape factor where for cylindrical pores but larger for other pore geometries (*Schlueter* *1995*). This relationship is only valid for uniform pore shapes and cannot account for the interconnected, tortuous, and non-uniform nature of natural porous media (*Hunt,* 2013). Refinements to this relationship have been made through the Kozeny-Carman relationship (*Carman*, 1937, 1939):

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|  |  | [11] |

From this relationship it is apparent that permeability is proportional to porosity and the square of the hydraulic radius. In addition, the hydraulic radius and tortuosity represent frictional forces in this empirical relationship because the hydraulic radius decreases for non-circular pores and the path length of flow increases for larger tortuosity values.

Porosity and hydraulic radius can be readily derived from image analysis of the segmented CT volumes, but this cannot easily be accomplished for tortuosity. Since tortuosity encompasses broad definitions in the literature—diffusive, geometric, hydraulic, and electrical tortuosity (*Ghanbarian et al. 2013*). We therefore evaluated six published methods for estimating tortuosity for the KC equation (*Boudreau, 1996; Yu and Li, 2004; Li and Yu, 2011; Matyka et. al., 2008; Koponen et. al., 1996; Iverson & Jorgensen, 1993*), due to their ease of calculation from image analysis data. An apparent limitation of the KC relationship is that a non-percolating soil sample can return , as long as a non-zero porosity, hydraulic radius and tortuosities are used in the model. Because LB simulations are guaranteed to yield zero permeability on non-percolating structures, KC estimates for such samples were excluded to make an unbiased comparison possible.

*2.6 Error Metrics*

Four error metrics were used to evaluate the correspondence between permeabilities generated with the LB or KC methods and those that were observed in the laboratory: mean error (ME), root mean square error (RMSE), unbiased root mean square error (URMSE), and a pearson correlation coefficient (r). These metrics were based on log10(k) because the laboratory permeabilities varied by more than three orders of magnitude. All errors are dimensionless.

ME was intended to quantify bias in the estimated permeabilities and was calculated according to:

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|  |  | [12] |

where *N* is the number of 1/8th sections for which the LB or KC methods could be applied; is predicted permeability, and is the measured permeability. A positive value of ME indicates that the simulations systematically overestimate permeability, while a negative value indicates underestimation. RMSE was calculated in a similar way:

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RMSE is statistically biased because it includes the systematic error quantified by ME. We therefore also calculated an unbiased RMSE according to:

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The pearson correlation coefficient (r) was used to quantify the correspondence in pattern between simulated and observed permeability. An emphasis for evaluation has been placed on the simulated 1/8th size sections because most segmentation methods produced non-percolating volumes for complete soil columns.

3 Results

*3.1 Segmentation Results*

Table 2 presents results of image analysis on the six segmentation results for Column 3 while Figure 2 shows the segmentation for section 2 of this column. Results for the other three columns or sections were qualitatively similar. Porosity values returned by the six segmentations spanned two orders of magnitude ranging from 0.2% (Brink) to 20% (IK), as shown in Table 2. Locally adaptive and clustering methods (IK, KM-MRF, and Otsu) return the highest porosity values. Due to the finite resolution of the CT scan (110μm), it was not expected that any of the segmentation would resolve the total all pore space which was derived from bulk density as 0.46 cm3/cm3. The soil water retention and soil pore distribution (Figure 1) indicate that more than 90% of the pore space is below the CT image resolution at less than 100 μm in diameter. The porosities returned by the Brink, Rosin, and Yen algorithms may provide better representations of macroporosity than those generated by IK, KM-MRF, and Otsu.

The IK, KM-MRF, and Otsu algorithms also yielded the greatest amount of pore space connectivity, as indicated by negative specific Euler numbers. These models also produced the highest hydraulic radii and lowest geometric tortuosity values. Considering the KC equation (Eq. 11) as a model for permeability, it can therefore be expected that the IK, KM-MRF, and Otsu segmentations will tend to yield much higher permeabilities than the Brink and, especially, the Rosin, and Yen algorithms.

With the exception of IK and KM-MRF methods most segmentations did not produce percolating columns for all of the 1/8th sections. It is possible that these sections are characterized by pores smaller than the current CT resolution, and that macropores do not traverse the entire length of the soil columns or even sections as was assumed during data collection. Given that measured permeabilities were always greater than zero, this implies that a significant amount of flow may have occurred through the unresolved pores in the matrix. Based on these suggestions it may therefore be necessary to image macroporous soils at a much higher resolution than 110 μm. This, however, would place much larger demands on CFD methods, which typically scale as with a power of the resolution. The segmentation algorithms that yield low porosities appear to yield more realistic pore structures but are less likely to percolate. Neither LB nor KC methods can deal with a possible matrix flow component (because these pores were not resolved).

*2.3.2 Permeability Derived by the Lattice Boltzmann Method*

Permeability results from the LB models appear in summarized form in Table 3. No results were obtained for the IK method owing to its extreme porosity, as discussed in the previous section. The large porosity, combined with the applied lattice pressure gradient caused flow rates caused numerical instabilities in the LB simulations. This could have been mitigated by using a smaller pressure gradient, but this was not pursued since the porosity of the IK method was unrealistically high making it unlikely that the IK method yielded a correct pore structure.

All methods yielded substantial ME, indicating that, on average, the LB method overestimated the permeability by 0.96 (Brink) to 2.32 (KM-MRF) orders of magnitude. Consequently large RMSE values are found for most segmentations, but URMSE results show that all methods had a much smaller variation around their mean value (0.78 to 1.09). Correlation coefficients (r) between were rather poor, varying between 0.37 (Brink) and 0.58 (Yen). It is worth pointing out that the “best” model in terms of ME (Brink), is the worst in terms of correlation coefficient.

Figure 3 shows most simulated permeabilities are indeed larger than those observed. While some segmentation methods yield LB permeabilities that are relatively close to the 1:1 line (Brink, Yen and to some extent, Rosin), the other segmentation methods yield permeabilities that are consistently too high (KMMRF, Otsu). The IK model would likewise have yielded extremely high permeabilities. We note here that the Brink and Yen segmentations have segmented porosities much smaller than 0.01 (Table 2), while the KMMRF, OTSU, Rosin (as well as IK) models have porosities that are much larger. Segmented porosity that is too large appears to play a major role in the overestimated permeability. Large porosities are also responsible for larger pore-connectivity as indicated by smaller (more negative) Euler numbers. The methods that perform the most poorly, have the smaller numbers. Comparison Table 2 shows that the methods with the smallest simulated permeabilities also have the largest tortuosities.

Figure 4 shows observed and simulated permeability profiles for Column 3. None of the segmentations provide a very compelling match with the observed profile of permeability – a finding that was already exhibited by low correlation coefficients. Even though they provided overestimations, the LB simulations appear to match the observations better when the observed permeabilities were above 10μm2. The correspondence between simulations and observations deteriorates for (observed) permeabilities below 10μm2 - with the exception of section 6 for which Brink and Yen yield comparatively good results. This pattern can also be found in Figure 3 which shows an increasing divergence of the LB permeabilities at lower observed permeabilities.

The general overestimation of permeability appears to suggest two things. Firstly, a matrix flow component was present in the observed permeabilities. The importance of this component decreases as the permeability increases due to the dominance of macropore flow. However, the relative importance of matrix flow would increase at lower observed permeabilities and since pores smaller than 110μm2 could not be resolved, the LB method could not account for this. Secondly, the volume or hydraulic radius of macropores that are revolved after segmentation are overestimated. Alternatively, it may be that tortuosity or wall roughness (which would tend decrease the hydraulic radius) are underestimated. This again, tends to confirm that higher-resolution CT scans would be preferable or, as discussed later, organic matter was present in the pores but was not detected by the CT method.

*2.3.3 Kozeny-Carman permeability models*

Porosity and hydraulic radius needed for the KC model can easily be derived from segmented volumes. Six tortuosity models evaluated as shown in abbreviated form in Table 4. To reduce the large number of segmentation and tortuosity permutations possible for KC evaluation (36) we selected the tortuosity model that returned the overall lowest (RMSE) in KC permeability, which was the *Li and Yu 2011*, a Sierpinski carpet pore fractal mode model given by:

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|  |  | [15] |

Table 5 shows the summarized results for the KC method in the same way as was shown in Table 5 for the LB method. In this case it was possible to evaluate the IK method, simply because the KC method does not require the computation of flow rates. Except for one method (Brink) all segmentation methods yielded positive ME, indicative of overestimation of permeability. The pearson correlations are dissapointingly low, with a Rosin and yen reaching values of 0.32 and 0.41, respectively. Correlation coefficients are especially poor for the other methods.

Figure 5 for all permeability and Figure 6 for the permeability profile of Column 3. Overall there is much weaker correspondence between observed and KC-estimated permeability than was observed for the LB method. Similar to the LB results, two groups of segementation exist in Figure 6. A high group is present that includes KM-MRF, Otsu, and IK which tends to over predict k. The low group and includes Brink, Rosin, and Yen. Neither group, however is able to match the trend in permeability for Column 3 (Figure 6). Similar results were found for the other columns, but are not shown here.

These results for the KC method suggest that image derived model data is not representing the same pore structure as was measured in the laboratory.

4 Discussion

*4.1 Variability in returned permeability values between segmentation algorithms*

The importance of the variability between automated segmentation algorithms cannot be overstated at this juncture. For example, Column 03 results display variation in porosity between 0.1% to 20% (Table 2). *Iassonov 2009* identified these wide ranging variations in porosity based solely on segmentation algorithm selection. Although porosity is not a main predictor of permeability, this variability also scales with large differences in connectivity as observed through specific Euler number (Table 2). A more negative specific Euler number is indicative of higher connectivity within the sample. It is also apparent that the tortuosity is inversely related to the porosity.

Modeled permeability results display the impact of this variability between segmentation practices commonly used in digital soil physics. The cases displayed in this study show variation of up to four orders-of-magnitude difference in permeability for LB models (Figure 3). LB models seem to follow a similar trend as laboratory data although the few matches in permeability seem to be more of a coincidence than model rigor. LB model permeability do not appear to scale directly with porosity or modeled tortuosity. Instead LB models are influenced directly by pore connectivity and a combination of factors including but not limited to porosity and tortuosity.

KC model tortuosity is directly calculated from porosity via equation 11. Two distinct groups of data are observed within the KC results. Higher porosity segmentation methods are defined as algorithms that returned mean porosity of greater than 5% porosity. These high porosity models return high permeability values and seem to follow a similar trend as each other. The lower porosity group of segmentation methods, return permeability values that are more similar to laboratory values and also follow a similar trend as one another. These methods still show significant variability between returned permeability values. It is obvious that the low permeability methods do not return trends that are consistent with the general trend displayed by the laboratory data (Figure 5). Extremely high tortuosity values in this group, 8.77 – 20.59, highly influence the results since permeability scales with . It is apparent that CT porosity is the controlling factor in the KC model because geometric tortuosity approaches infinity as porosity approaches 0. The variability observed here illustrates the direct influence to modeled permeability with modifications in modeled porosity and connectivity by applying different segmentation algorithms.

*4.2 Potential sources of uncertainty between modeled and measured permeability*

Many potential sources of uncertainty have been presented thus far and will be discussed with regard to this study. Common petrophysical laboratory methods such as gas permeameters are limited to making measurements of up to 10 ; these methods cannot produce representative permeability for macropore samples which are characterized by much higher flow rates (*Sukop 2013*). Options for measuring samples characterized by high flow rates include mega air permeameters (*Ferreira 2010*) and measuring outflow from constant head fluid methods (*Fetter 2001*) as in this study. Considering the relatively small amount of variation in the standard deviation (Table 1) of the laboratory measurements taken, it is unrealistic to assume that the differences in modeled permeability and laboratory measurements can be explained by standard laboratory error. It is shown that pore deformation and/or destruction may have occurred during the cutting process for column 7 and column 8. Laboratory results show slightly less than a 1:1 ratio between harmonic mean permeability and the permeability of the intact soil columns (Table 1).

Macropore deformation or destruction, which occurred *after* CT scanning but before the permeability measurements, may have resulted in alterations in the pore structure that were more significant than anticipated. Such changes would probably have yielded lower observed permeabilities that were consistently lower than would be consistent with the imaged column. Whole-column permeability measurements were conducted (Table 1), but could be replicated with LB only for a few of the segmentation methods (KM-MRF, IK) for all columns; all other methods yielded non-percolating sections at least in some of the columns.

A soil water characteristic curve was taken for a representative soil core from the same floodplain grazing site as columns 3, 7, 8, and 9. Pore-size distribution was modeled using equation 3 (Figure 1). Over 90% of the porosity is present in pores smaller than the image resolution (Figure 1) and can be classified as unresolvable micro-porosity. This suggests that macropores should be responsible for transmitting the majority of fluid through the simulations. However, laboratory permeability results returned values ranging from 0.02 to 32 . These are equivalent to hydraulic conductivity values ranging from a minimum of approximately 2.07x10-5 cm/s to a maximum of approximately 0.04 cm/s. The lower permeability values are consistent with those belonging to non-macroporous clay loams and silty clay loam textured soils. Permeability values above approximately 7 seem to be consistent with macropore flow based upon UNSODA and Soil Survey textural tables reported in *Leij et al.* *1999* assuming macropores percolate faster than sand. Only 14 sections in total of all 32 measured 1/8 sized soil sections reported laboratory permeability results greater than 7 . Laboratory permeability results for each soil column include at minimum one 1/8th size soil section with a permeability of less than 1 . This is inconsistent with macropore flow being main conduit for fluid flow through these tested soil column sections. This analysis is consistent with our observation that LB estimated permeabilities were “better” once the observed permeabilities were larger than 10 . It therefore appears that matrix flow controls the macro-porous flow through the columns.

It is also possible that organic matter (decomposed roots or fauna, such as earth worms) may have been present in the macropores of the samples. While large volumes of organic matter would have been noticed by the experimentators while curring the samples, it is possible that smaller pieces of organic matter obstruct critical hydraulic connections in the samples. Organic material present in the macropores of the sample may not have been resolved in the CT samples because low atomic mass elements such as H, C, N, and O are largely transparent to x-ray photon energies used in CT scanning (*Wildenschild 2002*). The hydraulic networks that were segmented by some of the low-porosity algorithms may therefore been accurate, but due to the presence of organic matter only partially active. Organic matter can be imaged using lower energy x-ray photons, but unfortunately these are blocked in soils due presence of more massive elements such as Si and Ca.

CT collection and image data are rarely perfect representations of the physical world, since they are disturbed by optical transfer functions, scattering, and noise (*Kaestner 2008*). Operator bias such as image resolution choice, exposure settings, beam energy, and flux may result in systematic errors in subsequent imaging processing steps (*Houston* 2013). Due to averaging of the attenuation of multiple materials or phases in a single voxel, partial volume effects may be present, and boundary voxels may be misclassified (*Ketcham 2001*). Misclassification of boundary voxels can significantly affect modeled permeability results. Visual inspection of three dimensional imagery of model pore networks—such as seen in Figure 2—support the possibility of voxel misclassification in some models. Column 3, section 2 is used as an example, because lattice Boltzmann simulations returned permeability values that are comparable to laboratory values. Differences in modeled permeability values between segmentation algorithms are influenced by partial boundary effects.

*4.3 Observed relationships between lattice Boltzmann and Kozeny-Carman models*

It is apparent that both LB and KC models tend to predict permeability within a similar range of variation from the laboratory data (Figure 3, Figure 5). Kozeny-Carman predictions, do not match 1:1 with lattice Boltzmann results. Instead KC models returned results with a much smaller RMSE permeability than LB (Table 3, Table 5). By using the assumption of , KC models assume perfectly cylindrical pores (*Carman 1927*). KC models predict permeability values that regularly 1-2 orders of magnitude less than lattice Boltzmann permeability results across all model results (Figure 7). At very low porosity, both LB and KC display significant changes in permeability values with small changes in porosity. The KC equation is more sensitive to these changes due to the large influence of the geometric tortuosity at low porosity values (Figure 8).

KC model permeability values are highly correlated with porosity (r2=0.59) (Figure 8). In the KC model porosity is included directly in the numerator, in the calculation of Tortuosity, and indirectly in the hydraulic radius calculation. LB model values correlate less strongly with porosity (r2=0.39). At permeability changes dramatically with very small changes in . For both modeling equations, small increases in porosity yields a smaller density of fluid particles contacting frictional surfaces (Figure 8). These types of increases may not generally be observed in natural systems, due to organic matter such as hummus and root mass providing additional friction surfaces in macropores. The models in this study behave more ‘pipe-like’, due to the inability of the collected CT data to resolve organic material. Although no optimization between LB and KC model results is applied, a strong correlation is observed in the permeability data (Figure 7). Power regression analysis of LB and KC results yields a relationship of . This is a notable relationship given the underlying assumption that all pores in the KC model are cylindrical.

5 Summary and Conclusions

The principal objective of this paper was to identify limitations of modeling permeability from CT data of natural macroporous media using image-based (KC) and and computational dynamics based (LB) methods. Simulation domains were generated from six different automated segmentation algorithms and compared to laboratory measurements in an effort to validate each model and gain insight into relationships between KC and LB models. Four macropore soil columns composed of 8 sections each were modeled using both KC and LB methods and were compared with laboratory measurements. We reach the following conclusions.

* We observed extreme variation in the pore structures returned by the six segmentation algorithms. Simple algorithms that set a global threshold consistently returned lower porosities than more sophisticated algorithms that used local information for voxel classification. It was found that low porosity segmentations were more likely to represent the macroporous structure present in the samples.
* Observed permeabilities were likely controlled by flow through the matrix. Pores smaller than the image resolution (110μm) were not resolved and neither LB nor the KC methods could account for matrix flow.
* Both KC and LB models returned permeability values that ranged from 2 orders of magnitude less than laboratory measured permeability values to 3 orders of magnitude greater than laboratory collected permeability values. In general we found a better correspondence between estimations and observations if the observed permeability was greater than 10 μm2.
* In general both methods overestimated permeability which suggests that the pore volume allocated macropores was too large. It is also possible that part of the resolved pore-space was blocked with organic matter (which cannot be resolved by CT) or that the pore structure was altered by deformation or smearing after cutting each column into eight sections. It is also possible that the imaging resolution used (110 μm) is inadequate to resolve all relevant pore features. The use of image higher resolutions would place higher demands on CFD techniques than image analysis-based techniques.
* For all segmentation methods LB-derived permeabilities had stronger correlations with the observed permeabilities than did the permeabilities obtained with the KC method. This implies that CFD-based methods are superior over KC-based methods that rely on image analysis.
* Even though the different segmentations yielded a large variation in porosity and pore structures, LB and KC estimates of permeability exhibited a stronger correlation with each other (r2=0.76) than the best correlation with observed permeabilities (0.56 for LB-Yen, and 0.41 for KC-Yen). This seems to imply that LB and KC are largely consistent even though they rely on different analysis methods (fluid flow versus image analysis). The relatively poor results of this study should not primarily be sought with these methods. Better estimates are more likely obtained by improving the quality of CT scans (better signal to noise ratio, improved resolution) or segmentation algorithms. It may also be necessary to choose a soil medium in which the flow is clearly dominated by macro-pore flow and is not a mix of matrix and macropore flow or caused by unresolvable obstructions.

## *Acknowledgements*

*This study was supported, in part, by USDA-NIFA, Project number ARZT-3007050-G21-521, Award number 2014-67019-21718.*

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## 7 List of Figures

Figure 1: Soil water characteristic for soil column 01 which is located in the same floodplain grazing site as C3, 7, 8, & 9 (left). Pore size distribution shows that over 90% of the total porosity is unresolvable at the current CT image resolution (right).

Figure 2: Three dimensional reconstructions of Column 03, section 02 illustrate the large variability in pore space representation between automated segmentation schemes. CT porosity values are Brink 0.018 (a), IK 0.297 (b), KM-MRF 0.147 (c), Otsu 0.238 (d), Rosin 0.050 (e), Yen 0.026 (f)

Figure 3: Lattice Boltzmann modeled permeability results for all four tested soil columns return values up to 5 orders-of-magnitude greater than laboratory collected permeability values

Figure 4: Lattice Boltzmann permeability models performed on eighth sized sections of soil column 03 returned results that that range 3 orders-of-magnitude depending on the segmentation algorithm used to binarize the initial CT data. With the exception of section 6, no models produced permeability results that validate with laboratory data.

Figure 5: Kozeny-Carman modeled permeability results for all four tested soil columns return values that range from 2 orders-of-magnitude less than to 2 orders-of-magnitude greater than laboratory collected permeability values.

Figure 6: Kozeny-Carman permeability models results formed two distinct groups based upon segmentation algorithm. Otsu, KMMRF, and IK follow similar trends forming a high k group. The remaining segmentation algorithms form a low permeability group. With the exception of section 2, no models produced comparable results to laboratory collected permeability.

Figure 7: KC permeability models return results that are regularly 1-2 orders-of-magnitude less than LB modeled permeability. A strong correlation , is observed.

Figure 8: KC models correlate more strongly with porosity than LB models. It is apparent that at small changes in porosity generally correlate with large changes in modeled for KC models . LB models display a similar, but less strongly correlated, trend .

## 8 Tables

Table 1: Harmonic mean permeability of cut sections show that pore deformation or destruction may have occurred for Column 7 and Column 8 since mean permeability measured from the intact soil column is more than the harmonic mean of the separate sections.

|  |  |  |  |
| --- | --- | --- | --- |
|  | *keq-n* | *km* | *SD km* |
| *Column 3* | 4.30 | 1.80 | 0.26 |
| *Column 7* | 0.64 | 0.80 | 0.07 |
| *Column 8* | 0.07 | 0.17 | 0.08 |
| *Column 9* | 2.66 | 0.22 | 0.05 |

Table 2: Specific Euler number as a metric of pore connectivity correlates directly with LB mean k except for the Brink segmentation method. KC mean K values correlate directly with mean tortuosity and porosity as is expected from equation 11.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Euler number | Porosity | Mean Tortuosity | RH | N |
| Brink | -438 | 0.002 | 17.10 | 0.35 | 6 |
| IK | -293316 | 0.200 | 2.17 | 0.76 | 8 |
| KMMRF | -56072 | 0.068 | 4.25 | 0.70 | 8 |
| Otsu | -854032 | 0.142 | 2.58 | 1.30 | 6 |
| Rosin | -16241 | 0.016 | 8.77 | 0.57 | 5 |
| Yen | -754 | 0.003 | 14.37 | 0.37 | 6 |

Table 3: Number of percolating columns, mean error and pearson correlation coeficients for lattice Boltzmann simulaitons.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | N | ME | RMSE | URMSE | r |
| Brink | 21 | 0.96 | 1.45 | 1.09 | 0.37 |
| IK | 32 | -- | -- | -- | -- |
| KMMRF | 32 | 2.32 | 2.48 | 0.87 | 0.45 |
| Otsu | 32 | 2.27 | 2.47 | 0.97 | 0.33 |
| Rosin | 30 | 1.78 | 1.95 | 0.79 | 0.58 |
| Yen | 28 | 1.57 | 1.78 | 0.83 | 0.56 |

Table 4: ME permeability for different tortuosity methods applied when calculating from the KC relationship shows that Li and Yu 2011 generally returns lower ME than other tested methods. Note that changes to the KC shape factor will alter these values.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | *Boudreau (1996)* | *Yu and Li (2004)* | *Li and Yu (2011)* | *Matyka et. Al. (2008)* | *Koponen et. al. (1996)* | *Iverson & Jorgensen (1993)* |
| Brink | *-2.94* | *52.16* | *-0.94* | *59.63* | *-1.04* | *76.84* |
| IK | *-1.66* | *53.82* | *-0.50* | *70.75* | *-0.60* | *106.87* |
| KM-MRF | *-1.57* | *41.64* | *-0.44* | *55.70* | *-0.53* | *85.56* |
| Otsu | *-1.90* | *49.77* | *-0.71* | *61.46* | *-0.82* | *87.37* |
| Rosin | *-2.31* | *59.10* | *-0.74* | *70.72* | *-0.84* | *96.74* |
| Yen | *-2.56* | *61.98* | *-0.77* | *72.78* | *-0.87* | *97.24* |

Table 5: Number of percolating columns, mean error and pearson correlation coeficients for the Kozeny Carman models

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | N | ME | RMSE | URMSE | r |
| Brink | 21 | -0.37 | 1.34 | 1.29 | 0.16 |
| IK | 24 | 2.00 | 2.47 | 1.44 | -0.01 |
| KMMRF | 32 | 1.91 | 2.19 | 1.07 | 0.16 |
| Otsu | 32 | 1.70 | 2.10 | 1.23 | 0.05 |
| Rosin | 30 | 0.80 | 1.33 | 1.06 | 0.32 |
| Yen | 28 | 0.30 | 1.12 | 1.08 | 0.41 |