Characterization and Modeling of Macro-pore Flow in Heap Leach and Waste Rock Material[1]

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ABSTRACT

To date, existing theoretical approaches, characterization methods and numerical modeling of unsaturated flow poorly describes material influenced by macro-pores. In an effort to better determine unsaturated flow behavior in gravelly materials, we have developed laboratory methods to directly measure unsaturated flow and moisture retention characteristic data. Laboratory experiments were conducted for waste rock material containing more than 50% gravel to obtain direct measurements of moisture retention characteristic, and saturated and unsaturated hydraulic conductivity data on bulk material (i.e. no gravel removed) and with the gravel fraction removed. Traditional and modified versions of the van Genuchten and Mualem function was used to fit the moisture retention characteristic and hydraulic conductivity laboratory measurements. In general, unsaturated flow parameters derived from the traditional approach could not accurately describe the measured unsaturated flow data. Numerical flow modeling of the experimental data was also conducted using the computer codes HYDRUS-1D and MACRO 5.0. MACRO 5.0 employs the modified van Genuchten and Mualem equation, and a kinematic wave function for macropore flow and was most successful in replicating unsaturated flow data. The direct unsaturated hydraulic conductivity measurement method and MACRO modeling approach are powerful tools which can more accurately describe the behavior of preferential flow in waste rock and heap leach facilities.

Additional Key Words: unsaturated hydraulic conductivity, moisture retention characteristic, gravel, van Genuchten and Mualem equation, kinematic wave function

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INTRODUCTION

The presence of gravel particles (> 4.75 mm diameter) can significantly affect the moisture retention characteristic (MRC) and unsaturated hydraulic conductivity function (K(θ) of soils. In particular, the typically gravelly nature of waste rock and heap leach material creates large macro-pores that can significantly affect flow and transport behavior of both solution and air within these materials. Some researchers have shown that increasing gravel content decreases the saturated hydraulic conductivity (K_s) (Bouwer and Rice 1984, Dunn and Mehuys, 1984), whereas others have shown that K_s can increase or decrease depending on the percentage of gravel fragments (Milczarek et al., 2006, Cousins et al, 2003, Poesen and Lavee, 1994). The water holding capacity of the gravelly soils tends to be smaller than that for the nongravelly soils at matric potential heads less than -100 cm (Milczarek, 2006, Khaleel and Heller, 2003). Air entry values have also been observed to decrease as gravel contents exceed 30 percent (Milczarek, 2006).

Typically, MRC and K_s data are obtained through laboratory experiments on the fine fraction (< 2 or 4.75 mm grain size) of the field-collected samples. These data sometimes are used directly without considering gravel effects. In other cases, correction factors are applied to the measured data to account for the effect of gravel on the MRC and K_s based on the volumetric or gravimetric gravel content. Several researchers have shown however (Milczarek et al. 2006; Cousin et al. 2003; Khaleel and Heller, 2003), that a simple correction factor can lead to highly erroneous estimates of the MRC relation and K_s.

For soils with a high percentage of gravel particles, the spatial distribution of the gravel can create macro-pores and discontinuity in the pore size distribution. Two or more distinct regions in MRC have been observed by several researchers (Milczarek et al., 2006; Al-Yahyai et al., 2006; Poulsen, 2002). Therefore, the MRC and K(θ) for the gravelly soils should require two or more functions to describe the unsaturated hydraulic properties for the entire pore-size distribution. Larsbo et al. (2005) proposed a dual-permeability model MACRO 5.0, in which the overall pore space is divided into macropores and soil matrix. A kinematic wave equation (Germann, 1985) is used to describe water flow in macropores, while the Richards' equation is used to simulate water flow in soil matrix. Most unsaturated flow models (e.g. HYDRUS, UNSATH, SWIM, and SoilCover) are limited to Richards' equation to describe water flow, however, the existence of macropores can lead to preferential flow which cannot be simulated by the Richards' equation.

In this paper, laboratory experiments were conducted for a gravelly soil to determine the MRC and K_s with the gravel included (bulk sample) and with particles > 4.75 mm diameter removed. In addition, direct K_{unsat} measurements were conducted at three known unsaturated flow rates for better prediction of the K(θ) relation. Unsaturated flow was then simulated using the computer code MACRO 5.0 and HYDRUS-1D to compare the best fitting methods and predictive results.

MATERIALS AND METHODS

A sample of gravelly soil (56% >4.75 mm particle diameter) was collected from a mine waste facility in northeastern Nevada. The sample was homogenized and two subsamples removed, one for bulk sample analysis of MRC, K_s and K_{unsat} and the second for MRC and K_s analysis with the particles > 4.75 mm in diameter removed.

For the bulk sample measurements particles retained by the 1 ½-inch sieve (38 mm) were removed and the sample was packed into a 30 cm diameter by 30 cm long core instrumented with tensiometers at depths of 10 and 20 cm, and a water content sensor at a depth 15 cm. Except for dry end measurements of the MRC, all hydraulic analysis (i.e. MRC, K_s, K_{unsat}) were performed in the column in the following order: 1) K_s measurements, 2) K_{unsat} measurements and, 3) MRC measurements. MRC was measured using a combination of hanging water column and pressure (Tempe) cell extraction methods (Dane and Hopmans, 2002). Dry end measurements of the MRC (matric potential heads < -7000 cm) were obtained via the chilled mirror method (Gee et al., 1992) on samples with particles retained by the #10 sieve (>2 mm) removed. The dry end MRC water content measurements were corrected for gravel content by assuming the gravel particles contributed no additional moisture content under very low matric potential heads (e.g. < -7000 cm). K_s was measured via the constant head method (Reynolds and Elrick, 2002) using hydraulic heads between 2 to 5 cm.

K_{unsat} values were measured using a long column approach (Corey, 2002). Water was applied through an evenly distributed network of 12 irrigation points at rates of approximately 2×10^{-3}, 2×10^{-4}, and 2×10^{-5} cm/sec to the surface, with an approximate matric potential head of -10 cm applied to the bottom of the core with a vacuum pump. Steady state water content conditions were achieved when matric potential head readings from the two tensiometers were similar. Approximately 3-5 days of drainage was allowed between the irrigation cycles. Water content and matric potential head changes during the irrigation/drainage cycles were recorded via the water content sensor and tensiometers, respectively, for modeling of water flow.

The other subsample was sieved to remove particles > 4.75 mm in diameter and packed into a 5 cm diameter by 18 cm long core for MRC and K_s measurements using the pressure cell and constant head method, respectively.

MRC and Unsaturated K Fitting/Estimation

MRC and $K(\theta)$ functions were developed from the measured MRC, K_s, and K_{unsat} data via five methods.

Method 1 - The standard van Genuchten (SVG) equation (van Genuchten, 1980) was fitted to the MRC data for the total range of pore sizes. The corresponding standard van-Genuchten-Mualem (SVGM) $K(\theta)$ relation (van Genuchten, 1980) was estimated using the optimized MRC fitting parameters, measured K_s, and a fixed shape factor, L, of 0.5.

Method 2 - The SVG equation and van Genuchten-Mualem unsaturated hydraulic conductivity model was fitted to the MRC and measured K_{unsat} data (SVGM with K) as a joint objective function for the total range of pore sizes. K_s was obtained from the best fit.

Method 3- The measured MRC on the < 4.75 mm diameter sample material was used to parameterize the SVG equation and the K(θ) relation was estimated from the SVGM model with measured K_s and L equal to 0.5.

Method 4 - Method 4 is the same as method 3 except that a gravel correction was made for the water content data using the equation of Gardner (1986):

$$\theta_c = \theta(1-\alpha) \tag{1}$$

where θ_c is the corrected water content and α is volumetric percentage of the gravel. A gravel corrected K_s was obtained using the equation of Bouwer and Rice (1984):

$$K_{cs} = K_s(1-\alpha) \tag{2}$$

where K_{cs} is the corrected K_s. The gravel corrected retention data and K_{cs} were then applied to the SVG and SVGM models to obtain the MRC function and estimated K(θ) relation.

Method 5 - The modified van Genuchten (MVG) equation of Vogel (2001) was fit to the MRC data excluding data at or close to saturation (> -5 cm matric potential head) to eliminate macropore flow effects. Parameters of the modified van Genuchten-Mualem (MVGM) equation by Luckner (1989) were then determined by fitting to the measured K_{unsat} data, while fixing the van Genuchten parameters to the previously determined values. The hydraulic conductivity function in macropores is given as a simple power law of the macropore degree of saturation, S_{ma}:

$$K_{ma} = K_{s(ma)} S_{ma}^{\ n^*},\ \theta > \theta_b \tag{3}$$

where $K_{s(ma)}$ is the saturated hydraulic conductivity of the macropores, and n^* is a "kinematic" exponent reflecting macropore size distribution and tortuosity.

The computer program RETC4 (van Genuchten et al., 1991) was used to fit the experimental data using methods 1, 2, 3, and 4. For method 5 the MRC function was fitted in RETC4 while fitting of the K(θ) function was conducted with a spreadsheet model.

Unsaturated Flow Modeling

Unsaturated column outflow experiments at the 2×10^{-4} cm/s irrigation rate were simulated with computer codes HYDRUS-1D (Simunek et al., 1998) and MACRO 5.0 (Larsbo et al., 2005). Parameters obtained using MRC and K(θ) fittings/estimation methods 1 through 4 were used to parameterize HYDRUS-1D. HYDRUS-1D does not have an option to implement the MVGM equation, thus unsaturated flow modeling using MRC and K(θ) functions parameters from method 5 were done using MACRO 5.0 (Larsbo et al., 2005).

A 30 cm long one dimensional model domain was defined. The model domain was discretized into 200 nodes with node distances ranging from 0.14 to 0.3 cm. Initial conditions were defined based on the observed water contents. During irrigation a constant flux top boundary condition of 2.08×10^{-4} cm/s was assigned; during drainage the top boundary condition was zero flux. The lower boundary condition was set as free drainage.

RESULTS AND DISCUSSION

MRC and Unsaturated K Fitting/Estimation

Figure 1 shows the measured MRC data and the fitted MRC functions using Methods 1-5.

Table 1 lists the fitted SVGM and MVG parameters and the measured or fitted K_s. The MRC measured data for samples with and without gravel particles deviate substantially from one another, indicating a significant influence from gravel content on the MRC. Correction of water content to account for the removed gravel fraction resulted in better agreement in MRC data between the bulk sample and #4 sieved sample at low matric potential heads, however, the deviation increases at intermediate and greater heads. It should also be noted that measured water content values did not appear to reach equilibrium in the bulk sample at matric potentials < - 10 cm, possibly due to low hydraulic conductivity and reduced pore connectivity.

The fitted MRC functions for the bulk sample is similar when fit using Methods 1 and 2 (SVG and SVGM w K). The fitted MRC functions using method 5 (MVG) show no significant difference from Methods 1 and 2 at intermediate and low matric potential heads, but differ at high (near zero) heads. This result is expected given that the MVG method excludes matric potential data from near saturated conditions and assumes a lower saturated water content.

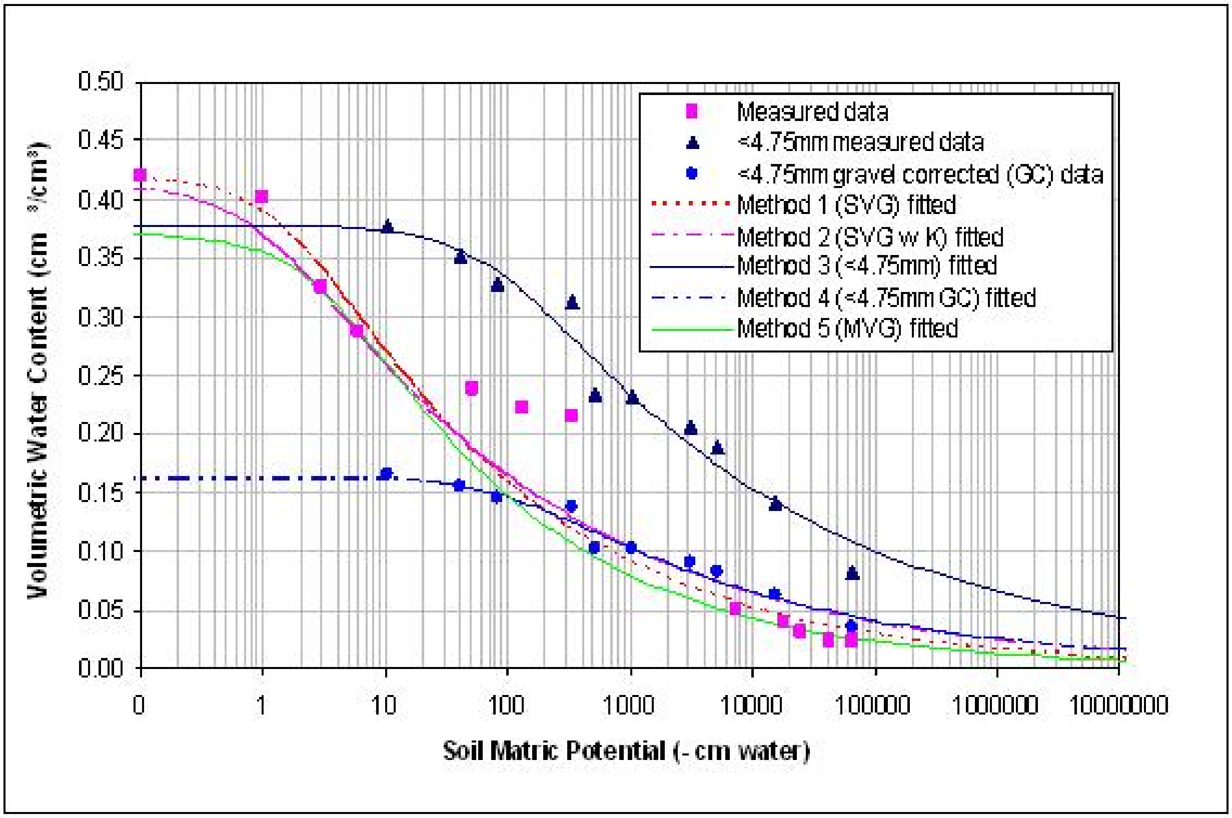

Figure 1. Measured and fitted soil MRC. GC = gravel corrected.

Table 1. Fitted van Genuchten-Mualem and modified van Genuchten-Mualem parameters and fitted/measured K_s.

Method	Saturated Hydraulic Conductivity (cm/s)	Unsaturated Hydraulic Parameters (van Genuchten parameters)				
		Residual Water Content (cm^3/cm^3)	Saturated Water Content (cm^3/cm^3)	α (cm^{-1})	N (-)	L (-)
1 – SVGM	>5.6E-2[a]	0.000	0.422	0.565	1.238	0.500[b]
2 – SVGM w K	6.6E-01[c]	0.000	0.413	0.903	1.20	0.000
3 - < 4.75 mm SVGM	>3.5E-02[a]	0.003	0.378	0.012	1.190	0.500[b]
4 - < 4.75 mm gravel corrected, SVGM	1.5E-02[d]	0.000	0.164	0.009	1.198	0.500[b]
5 - MVGM[e]	2.1E-04	0.000	0.312	0.314	1.267	7.217

[a] Beyond apparatus measurement capacity

[b] Fixed value

[c] Fitted saturated hydraulic conductivity

[d] Gravel corrected Ks

[e] Parameters for soil matrix in Vogel (2001) function

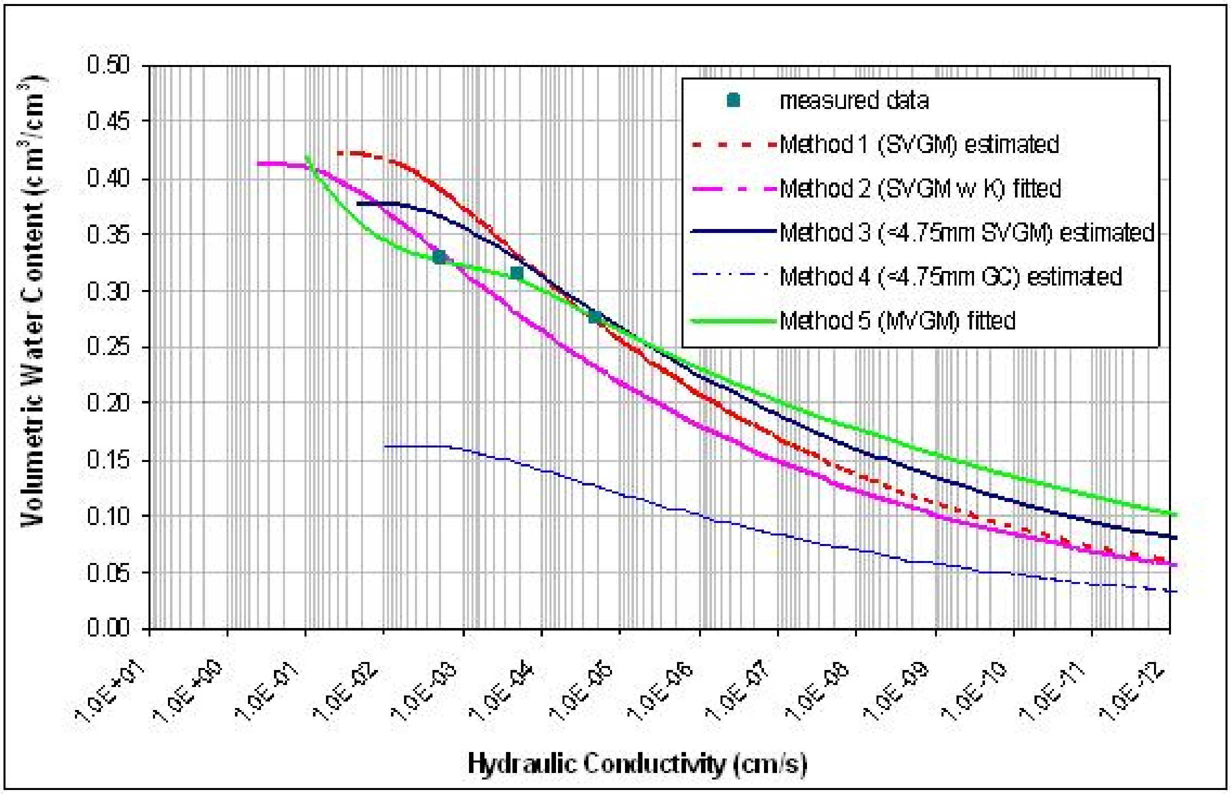

Figure 2. Measured and estimated or fitted K(θ). GC: gravel corrected.

Figure 2 shows measured, estimated and fitted K(θ) relations. The estimated K(θ) using Method 1 (SVGM) and Method 3 (<4.75 mm SVGM) reasonably approximated the measured K_{unsat} at the lower water content, but both diverge from the measured data as the water content increases. Method 2 (SVGM w K) provides an improved fit at the wettest measured K_{unsat} point, but significantly overpredicts K_{unsat} at the other two measured points. Method 4 estimated K(θ) relations for the gravel corrected < 4.75 mm particle diameter sample showed poor agreement with the measured bulk sample data. Method 5 (MVGM) showed the best agreement with the measured K_{unsat} data under the assumption that macro-pores and the soil matrix partition correspond to a water content of 0.31 cm^3/cm^3 and soil matric potential head of -3 cm.

Unsaturated Flow Simulation Results

Figure 3 shows the observed water contents during the unsaturated flow experiment and the HYDRUS-1D and MACRO 5.0 model simulated water contents using corresponding parameters obtained by Methods 1, 2, 3, and 5. Simulations using the gravel corrected derived parameters (Method 4) were not carried out due to the gravel corrected saturated water content being smaller than the observed initial water contents. Additional input parameters required for implementing Method 5 (MVGM) using the MACRO 5.0 model were a total K_s and porosity (both macropores and soil matrix) of 0.1 cm/s and 0.42, respectively, and n* (equation 3) of 2.0.

In general, the Method 1, 2, 3, and 5 simulations accurately predicted the wetting front arrival time and the initial drainage time, however, the predicted water content during irrigation and drainage rates varied considerably. The method 1 (SVGM) simulation overestimated water content at unit gradient conditions and also overestimated the drainage rate. That is, the simulations predicted a faster decrease in water content during the drainage phase than observed.

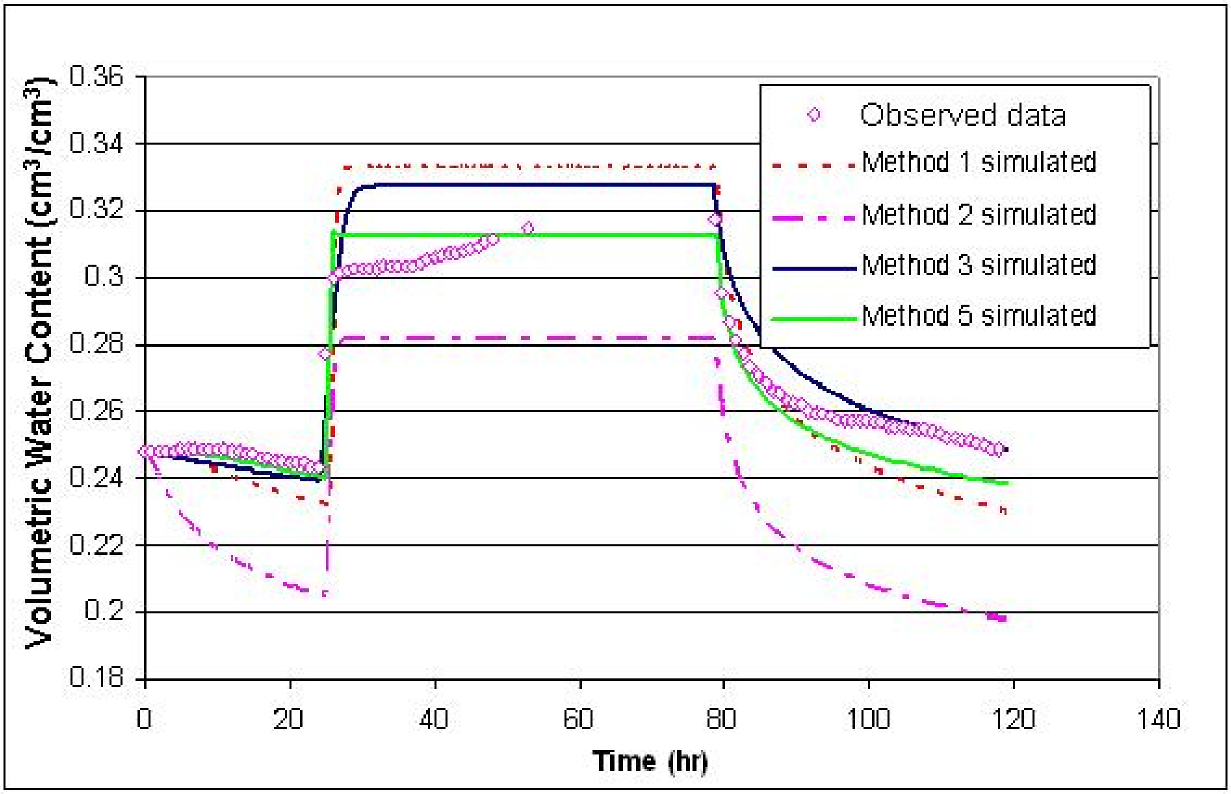

Figure 3. Measured water content during irrigation experiment and simulated values using parameters from Methods 1, 2, 3, and 5.

The method 2 (SVGM w K) simulation underpredicted water content during irrigation, but overpredicted the drainage rate. The method 3 (SVGM parameters from < 4.75 mm material) simulation over estimated water content and drainage rate. Method 5 (MVGM) simulation results were in better agreement with the observed water contents than the results from Methods 1 through 3 simulations, however, similar to the other methods it overpredicted drainage rate.

To assess the accuracy of the methods in modeling the matric potential heads during irrigation and drainage, the head data collected at 10 cm from the top of the column during the column outflow experiment was compared against simulated results using Methods 1, 2, 3 and 5. Figure 4 shows that the simulated matric potential heads do not agree with observed data during the transient flow periods, but reasonably predict matric potential heads during steady-state conditions. Most noteworthy were the simulated matric potential heads using Method 3 (SVGM parameters from < 4.75 mm material) which differed from the measured data by 3 to 4 orders of magnitude (data not shown). This behavior is explained by the hugely contrasting measured MRC data between the bulk sample and sample without gravel particles (Figure 1).

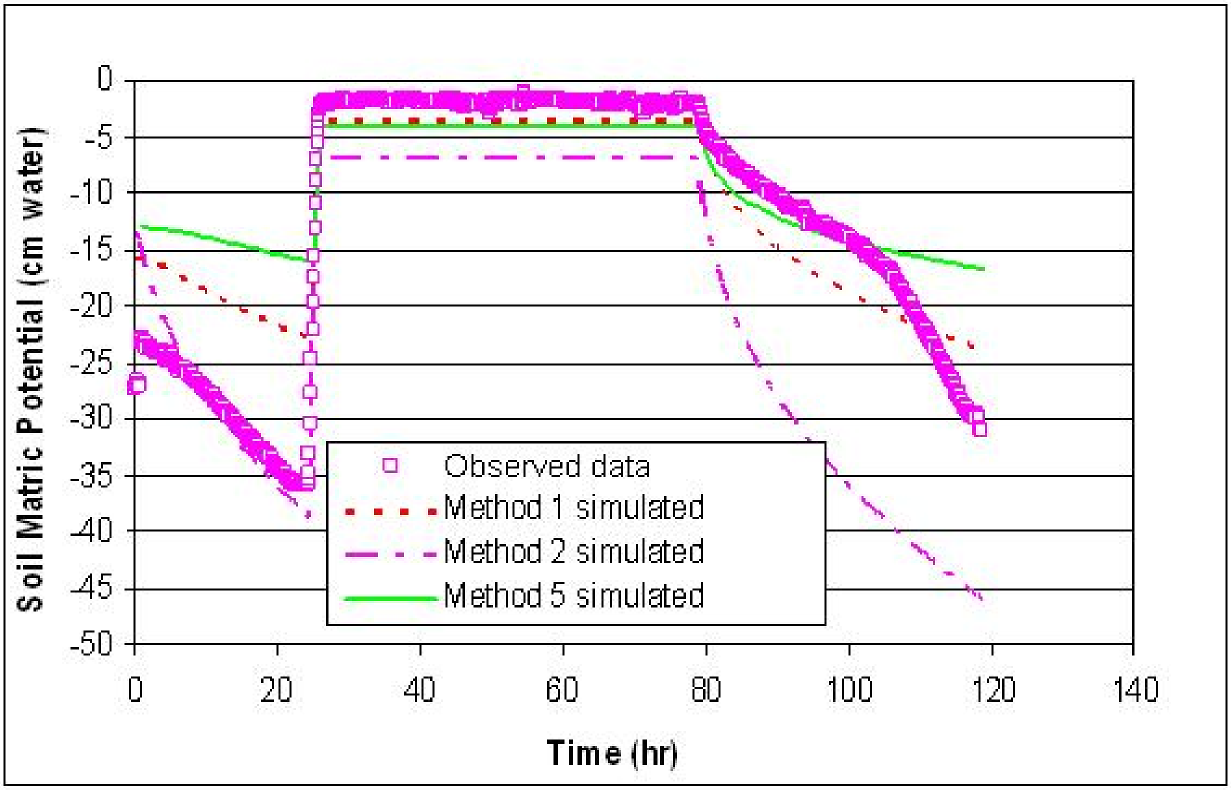

Figure 4. Measured matric potential heads during irrigation experiment and simulated values using parameters from Methods 1, 2, and 5.

Table 2 lists the performance of the different methods used to fit the MRC data and fit or estimate the K(θ) relations, as well as the performance of the parameters when used in simulations of unsaturated flow. The performance levels (i.e., poor, average, better, best) are relatively defined according to the calculation results of the root-mean-square error (RMSE), in which the RMSE of K(θ) fittings was calculated with the log-transformed values of the measured and predicted K_{unsat}. Among the five procedures, Method 5 (MVGM) showed the best performance for representing the MRC and K(θ) relations as well as simulating the outflow experiments with MACRO 5.0. Methods 4, which relied on MRC measurements using the < 4.75 mm size fraction and gravel corrected parameters, generated the worst performance. In representing the K(θ) relation and simulating water content during the outflow experiments, Method 3 (SVGM without gravel) generally outperformed Methods 1 and 2 which relied on the bulk sample. However, Method 3 performed significantly worse than Methods 1, 2, and 5 in simulating observed matric potential during the outflow experiment. The failure of agreement between the observed and predicted data from Methods 3 and 4 indicates that removing the gravel fraction from gravelly soil material results in unreliable representations of the MRC, K(θ) and K(h) functions. Additionally, the failure of agreement between the Methods 1 and 2 simulated and observed data suggests that a dual-permeability model is needed to accurately represent flow characteristics in gravelly material.

Table 2. Relative performance of each method in MRC and K(q) fitting or estimation and unsaturated flow modeling. Associated RMSE are in parenthesis.

Method	MRC Fitting	K(θ) Fitting/Estimation	Water Content Simulation	Matric Potential Simulation
1 - SVGM	Average (0.037)	Average (0.639)	Average (0.021)	Average (6.202)
2 - SVGM w K	Average (0.041)	Average (0.633)	Poor (0.040)	Average (10.249)
3 - SVGM w/o gravel	Poor (0.088)	Better (0.581)	Better (0.012)	Poor (>100)
4 - SVGM w/o gravel, w/ gravel correction	Poor (0.125)	Poor (NA)	Failed	Failed
5 - MVGM	Average (0.047)	Best (0.049)	Better (0.013)	Average (8.745)

NA: not applicable, indicates no fitted/estimated data at a given water content

CONCLUSIONS

Direct unsaturated flow and MRC experiments with gravelly waste rock material packed into large diameter columns showed significant differences in unsaturated flow and MRC properties in the same material where gravel had been removed. A modified van Genuchten-Mualem equation, which discretizes pore space into matrix and macropore flow, best represented the measured K(θ) relation and observed outflow experiment conditions for a gravelly soil. Predictions based on van Genuchten parameters derived from soil with the gravel removed or that did not utilize a dual-permeability model substantially deviated from the measured K(θ) and observed outflow data. These results indicate that accurate characterization of gravelly material requires inclusion of the gravel during hydraulic property measurements and that direct measurement of K_{unsat} along with the use of an appropriate duel-permeability model can more accurately describe the behavior of flow in gravelly waste rock and heap leach material.

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