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Comparison of different estimation procedures for the hydraulic properties of horticultural substrates by One-Step technique

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Abstract

The improved iterative method for the simultaneous determination of the hydraulic properties of growing media from One-Step experiment by Bibbiani, is performed and compared with simplified equations by Valiantzas and Londra. Brooks and Corey equation for water retention, and Kozeny power equation for hydraulic conductivity characterized the hydraulic properties of the porous media. The iterative procedure is applied on pure peat, pumice, and their mixes. The One-Step method has been previously optimized: processing the mean cumulative outflow curves recorded versus time, an estimation of diffusivity, and therefore of the hydraulic functions, is derived. Estimated water retention curve is compared with nine experimental data, and with the estimation of the Van Genuchten model, via the RETC code. Bibbiani's and Van Genuchten's models overlap except for the "very wet" range near saturation, whereas the Valiantzas and Londra's procedure didn't get satisfactory results. In regard to diffusivity, a good similarity between Bibbiani's and Van Genuchten-Mualem's curves can be assessed, while Valiantzas and Londra's procedure generally results in higher values. Due to the lack of estimation of the water retention curve, Valiantzas and Londra's procedure fails to estimate the hydraulic conductivity function, whereas Bibbiani's and Van Genuchten-Mualem's curves match together in most cases.

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Introduction

Water flow and solute transport modelling must rely on the knowledge of water retention and hydraulic conductivity curves, namely (h) and K(θ) or K(h). Computed water balances are very sensitive to soil hydraulic parameters and therefore their accurate determination is essential (Jhorar *et al*., 2004; Schneider *et al*., 2009). Experimental methods have been set for this task, with varying complexity and accuracy of measurements. The substrate moisture retention curve is rather easily achieved. On the contrary, the determination of the hydraulic conductivity function requires the establishment of steady-state moisture profiles under unsaturated conditions, which is a tough assignment. This difficulty led scientists to conceptual models which could predict K(θ) from the moisture retention curve coupled by Ks measured independently (conductivity at saturation, where simple permeameters have been manufactured either constant head or falling head). Gardner (1962) introduced another method which relies on the determination of diffusivity D(θ) relationship with one-step outflow data, being diffusivity the ratio of conductivity to the specific water capacity C(h)=d /dh. Henceforth, many authors developed more accurate equations.

In this paper the cumulative outflow data obtained by one-step outflow experiment are used for the prediction of D(θ) employing equations from Valiatzas (1989), Bibbiani (2002), Valiantzas *et al*. (2007), Valiantzas and Londra (2012), and Van Genuchten-Mualem model (Mualem, 1976; Van Genuchten, 1980). Bibbiani's method, assuming a particular power form with a small number of parameters for the θ(h) and K(h) curves, leads to the estimation of the hydraulic characteristics. The estimated hydraulic functions are compared with experimental data, and with the Van Genuchten-Mualem model curves.

Materials and methods

Five replications of peat, pumice, and a peat/pumice (1Pe:1Pu) [1:1 (v/v)] mix were packed in 347.5 ml cylindrical aluminum tubes (7.6 cm in diameter, 7.6 cm in height). The pumice is a 'tout-venant' material sieved at 8 mm maximum particle size. At the end of the procedure, the substrate samples were seated on a grid for a 30 minutes 'free drainage'. Samples were then weighed to determine the water content θ_{fd}. At this time, samples were subjected to the One-Step procedure. Firstly, they were seated on the porous plates of Buchner filter funnels with an air-entry pressure > 16 kPa and a plate conductivity equal to 2.28 cm/hr. An airtight lid was placed on the top of each funnel and a positive air pressure was applied. An initial pressure equal to -1 kPa referred to the core centre was applied; once equilibrium was reached, the core was weighed and replaced in the funnel, and a sudden application of a positive gas pressure increment marked the initiation of the outflow process recorded with time until equilibrium at the new pressure. The couple of pressure [-1;-10] kPa was chosen as it was the most accurate (Bibbiani, 2002). A duration of 48 hours proved to be sufficient to allow for the necessary equilibrium and calculations. To make a comparison with experimental moisture retention data, the above samples were resaturated: a drying retention curve was determined applying -1.0; -2.0; -3.0; -5.0; -10.0; -15.0; -23.0 kPa matric potential referred to the core centre. After -23.0 kPa measurement, the samples were removed and put in a ventilated oven at 105 °C for 24 hours and weighed. Then, the cylinder was clamped in a constant volume air pycnometer device to determine the total porosity θ_{TP}. To measure saturated hydraulic conductivity, the modified constant head method described by Da Silva (1991) was followed in its main steps using Plexiglas™ cylinder (20.0 cm in height and 5.1 cm in diameter). The process was replicated three times. The mean value was taken as the saturated hydraulic conductivity Ks.

In order to calculate D(θ) function, Valiantzas (1989) derived an accurate equation, starting from Gardner (1962) and Passioura (1976) approximate equations, as:

$$D(\theta) = -\frac{2 \cdot L^2}{\pi^2}\left(\frac{dq}{d\theta} + \frac{q}{\theta - \theta_f}\right) \tag{1}$$

where q = dθ/dt is the outflow rate, θ_f is the final volumetric water content in One-Step experiment, and L is the height of the sample. Valiantzas *et al*. (1988), and Valiantzas and Kerkides (1990) proposed a simple method for the simultaneous determination of hydraulic properties starting from an estimation of diffusivity function D(θ). Bibbiani (2002), in order to remove the limitation due to the absence of the θr parameter, re-introduced the latter in the relative water content equation. Thus, the proposed Θ equations are written as:

Brooks and Corey's (B&C, as referred herein after), for water retention

$$\Theta = \left[\frac{He}{h}\right]^{\lambda} \qquad h > He \tag{2}$$

$$\Theta = \frac{\theta - \theta r}{\theta s - \theta r} = 1 \qquad 0 \leq h \leq He \tag{3}$$

Kozeny's (KO, as referred herein after), for conductivity

$$Kr(\Theta) = \frac{K(\Theta)}{K_s} = (\Theta)^p \tag{4}$$

where θs is the saturated water content, θr is the residual water content, He is the air-entry value, p and λ are fitting parameters.

Eqs. 2, 3, and 4 can be substituted for D(Θ) equation obtaining:

$$D(\Theta) = B \cdot (\Theta)^A \tag{5}$$

$$B = \frac{Ks\,He}{\lambda(\theta s - \theta r)} \tag{6}$$

$$A = p - 1 - \frac{1}{\lambda} \tag{7}$$

The problem appears as an identification problem of parameters A, B, λ, and θr, while θs is taken as a known parameter, and calculated in this paper as:

$$\theta s = \frac{3\theta_{TP} + \theta_{fd}}{4} \tag{8}$$

The outflow rate q(θ(t)) is related to diffusivity D(θ) by approximate analytical expressions, λ (μ) and $\theta_L(\mu)$, μ depending on (θ; θr; A), as proposed by Valiantzas and Kerkides (1990) and modified by Bibbiani (2002):

$$q(\theta) = \frac{B\lambda^*(\mu)}{(A+1) \cdot L^2 \cdot (\theta s - \theta r)^A} \cdot [(\theta_L(\mu) - \theta r)^{A+1} - (\theta f - \theta r)^{A+1}] \tag{9}$$

Each θr value leads to estimate parameters A and B minimizing the difference between simulated and measured outflow rates q(t). Consequently the D(θ) function is calculated. Then, the unknown parameter λ is estimated minimizing the S(θr,λ) objective function, which is the difference between the natural logarithm of measured and simulated relative water content data, calculated as:

$$S(\theta r,\lambda) = \sum_{y=1}^{M} \{\ln[\frac{\theta_y - \theta r}{\theta s - \theta r}] - \lambda \cdot \ln[\frac{\lambda(\theta s - \theta r)}{Ks} B_{(\Theta)C}] + \lambda \cdot \ln[h_y]\}^2 \tag{10}$$

where M means number of experimental θ(h) data, θ_y is the water content in correspondence with h_y value of matric potential.

Thus, the minimum value function S(θr,λ) can be plotted, and its minimum singles out the best fitting vector [θ_r, λ_r]. Eq. 6 and 7 give parameters He and p, and so functions θ(h) and K(h) are plotted. In order to neglect the porous plate impedance effect on the results, which might be significant at the early stages of the outflow process, Valiantzas *et al*. (1988) forced the procedure for estimating D(θ) analyzing only the part of the curve where the cumulative outflow V ceases to be linear with respect to the square root of time √t. Later on, Valiantzas *et al*. (2007) and Valiantzas and Londra (2012) derived some simplified equation for the determination of the hydraulic properties of horticultural substrates, applying respectively Eq. 1 in the former, and B&C equation and Burdine model (Burdine, 1953) in the latter; they introduced in Eq. 1 a new dimensionless variable obtained from the outflow data as well, the fraction of the remaining outflow water volume S_{out}, as:

$$S_{out} = \frac{\theta - \theta_f}{\theta_i - \theta_f} = F(\sqrt{t})^G \tag{11}$$

which is related to cumulative outflow V vs. the square root of time √t with a power form similar to that of Eq. 5, where θ_i and θ_f are respectively the initial and final volumetric water content in One-Step experiment, F and G are fitting parameters. In this context, they derived the following:

$$D(\theta) = -\frac{2 \cdot (G-1) \cdot L^2 \cdot F^{2/G}}{\pi^2}\left(\frac{\theta - \theta f}{\theta i - \theta f}\right)^{-2/G} \tag{12}$$

In order to evaluate the hydraulic functions, they proposed to measure experimentally the water retention, or alternatively, in their latter paper, to run the One-Step procedure fixing θ_f as close as possible to the 'real' θ_r value.

In the present paper, in order to compare all the previous estimated water retention and hydraulic conductivity curves, the Van Genuchten–Mualem (VG-M, as referred herein after) combined model (Mualem, 1976; Van Genuchten, 1980) was applied to experimental retention data, having fixed their parameters respectively as m=1-1/n, l=0.5, and θs from Eq. 8. The fitting program RETC (Van Genuchten *et al*., 1991) estimated θr, α, and n unknown parameters, computing both experimental retention data coming only from One-Step experiment and diffusivity data calculated by Eq. 5.

$$\Theta(h) = \frac{\theta - \theta r}{\theta s - \theta r} = \left[1 + (\alpha \cdot |h|)^n\right]^{-m} \quad (13)$$

$$C(\Theta) = \alpha n m(\theta_s - \theta_r)\Theta^{1/m}\left(1 - \Theta^{1/m}\right)^m \quad (14)$$

$$K(\Theta) = Ks \cdot \Theta^{1/2}\left[1 - \left(1 - \theta^{1/m}\right)^m\right]^2 \quad (15)$$

$$D(\theta) = \frac{K(\theta)}{C(\theta)} \quad (16)$$

Finally, RETC code estimated D(θ) taking as input only 9 experimental moisture retention data, thus resulting in the VG-M (Retention only) curve.

Table 1. Water retention data-sets, and One-Step pressure heads set-up.

Pure Peat		1Peat:1Pumice		Pure Pumice	
Pressure Head h	Water Content θ	Pressure Head h	Water Content θ	Pressure Head h	Water Content θ
3.8 = 'θfd'	0.879	3.8 = 'θfd'	0.729	3.8 = 'θfd'	0.465
3.8 = 'θfd'	0.879	3.8 = 'θfd'	0.729	3.8 = 'θfd'	0.465
20	0.501	20	0.525	20	0.380
30	0.435	34	0.471	30	0.370
50	0.379	50	0.447	50	0.364
104 = 'θf'	0.329	104 = 'θf'	0.395	100 = 'θf'	0.347
140	0.318	147	0.376	140	0.340
230	0.309	233	0.361	230	0.335

Table 2. Measures parameters at saturation, and parameter estimation obtained for Eqs. 2-7. B&C-KO model.

Substrate	ρ kg m^{-3}	θ_{TP} m^3m^{-3}	θs m3m^{-3}	Ks cm min^{-1}	$\bar{\theta}_r$ m^3m^{-3}	A($\bar{\theta}_r$, λ) -	A($\bar{\theta}_r$, λ) -	λ -
Peat	115	0.94	0.92	3.360	0.298	2.7498	33.8752	1.1285
1Pe:1Pu	307	0.86	0.83	1.44	0.206	6.1897	19.715	0.3315
Pumice	830	0.68	0.62	180.0	0.248	6.827	100.75	0.1665

Table 3. Parameter estimation obtained for Eq. 12. Nonlinear least-squares analysis by RETC program (l = 0.5). Fit of 9 experimental retention data only for Eq. 13. VG-M (Retention only) model. Simultaneous fit of Retention and Diffusivity data from One-Step experiment for Eq. 13. VG-M model.

	Pure Peat		1Peat:1Pumice		Pure Pumice	
Variable	Value	St.dev.	Value	St.dev.	Value	St.dev.
Parameter for Eq. 12						
F	6.793		10.13		324.2	
G	-1.767		-1.433		-2.439	
Fit of 9 experimental retention data only for Eq. 13						
θr	0.3030	0.0058	0.2907	0.0102	0.3283	0.0091
α	0.1042	0.0030	0.2348	0.0113	0.8385	0.2135
n	2.3396	0.0700	1.5093	0.0298	1.6297	0.1234
m	0.5725		0.3374		0.3864	
R2	0.9993		0.9995		0.9964	
Simultaneous fit of retention and diffusivity data from One-Step experiment for Eq. 13						
θ_r	0.3072	0.0007	0.3069	0.0074	0.2788	0.0040
α	0.0984	0.0015	0.7149	0.0782	2.7400	0.1434
n	2.3681	0.0244	1.3873	0.0221	1.2906	0.0093
m	0.5777		0.2792		0.2252	
R^2	0.9993		0.9541		0.9923	

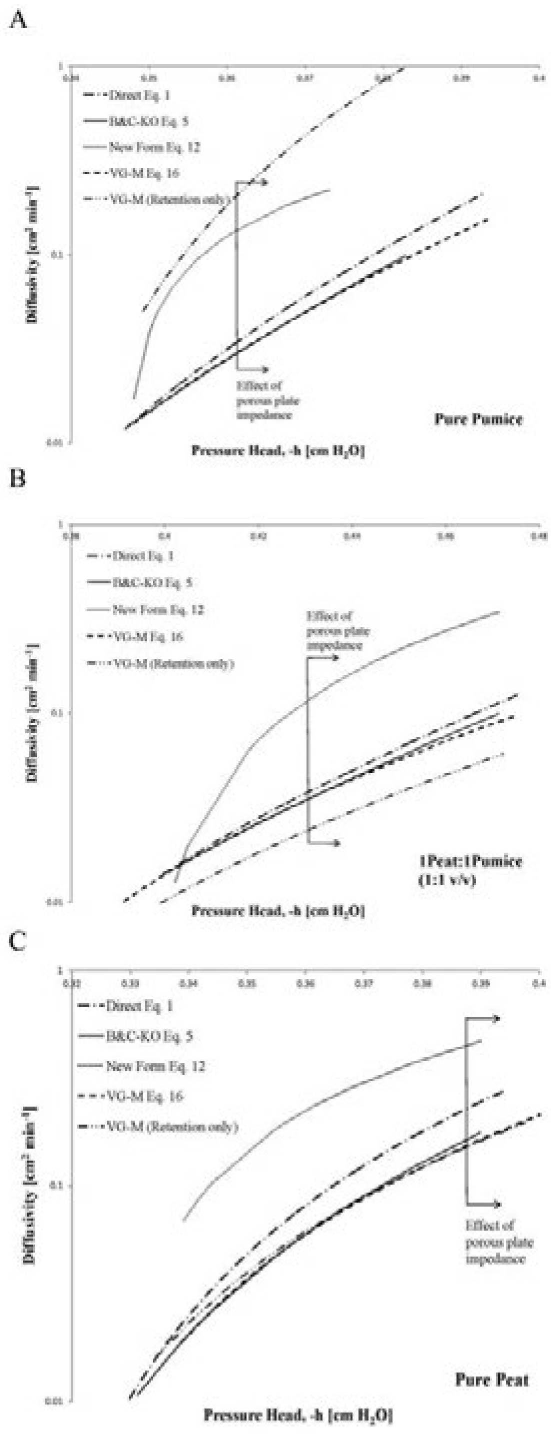

Figure 1. Substrate water diffusivity as a function of volumetric water content, D(θ), estimated by various equations. (A). Pure Pumice (B). 1Peat:1Pumice (1:1 v/v) (C). Pure Peat. The short vertical line labeled “Effect of the porous plate impedance” defines the region where the plate impedance is not negligible.

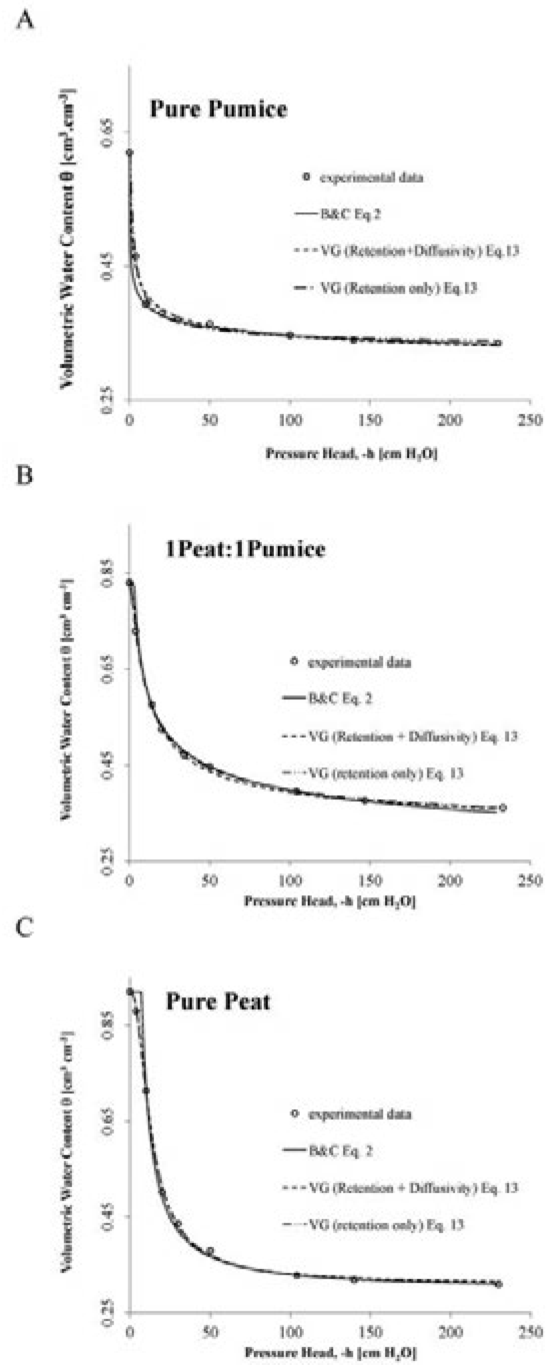

Figure 2. Substrate water retention θ(h) as a function of pressure head -h, measured and estimated by B&C and VG equations. (A). Pure Pumice (B). 1Peat:1Pumice (1:1 v/v) (C). Pure Peat.

Results and discussion

Table 1 reports all the measured moisture retention points for the three substrates, and the initial and final pressure heads set-up for One-Step experiment. Table 2 shows the estimated parameters for Eqs. 2 and 5, as related to the B&C-KO model improved by Bibbiani (2002).

Table 3 refers to Eq. 12, giving parameters of the new dimensionless variable S_{out}, obtained by Valiantzas *et al*. (2007). Moreover, it reports the estimation by RETC code for the VG-M model related to Eq. 13, with the analysis of 9 retention data only (derived from independent measurements), and both retention and diffusivity data derived from One-Step experiment. A comparison of diffusivity functions, $D(\theta)$, estimated by the above discussed equations, is well-drawn in Figure 1. Irrespective to the substrate nature, there is a good agreement between the direct calculation of $D(\theta)$ by Eq. 1, and both the B&C-KO model by Eq. 5 and the VG-M model by Eq. 16 (retention and diffusivity data). The VG-M (Retention only) curve shows a variable and unpredictable behavior, suggesting a non-reliable estimation based only on retention data. The prediction of $D(\theta)$ by Eq. 12 doesn't match any other ones in this experiment. Since Valiantzas *et al*. (2007) reported a substantial identity between their estimation and Eq. 1, the huge discrepancy in the present work might depend on the different final pressure at the end of the outflow procedure $h(\theta_f)$ that they fixed in the range -14÷-18 kPa. Doing this way, they assumed that θ_f is very close to the θ_r value, thus letting the estimation of θ_r^0; on the contrary, in this paper, $h(\theta_f)$ was chosen by analogy to the well-known tension range for the calculation of the hydraulic properties of horticultural substrates, such as the 'easy available water' value. On the basis of these results, the comparison of the water retention function gives us a deeper understanding of the whole estimation capability. Figure 2 shows the experimental data, the B&C and VG plot of the function, as well. As one can see, the main difference between B&C Eq. 2 and VG Eq. 13 estimated curve lies in the very wet range (i.e. $h(\theta)$<-1 kPa), being all the rest almost overlapped. Both the predictions by Valiantzas *et al*. (2007) and Valiantzas and Londra (2012) don't match the experimental water retention results (data not shown), most likely because of the same reason above explained. Moreover, the B&C Eq. 2 model, related only to One-Step procedure, seems to have the same power of estimation of the VG Eq. 13 model, both of them being in optimal agreement with the experimental water retention data.

Figure 3 provides us information about the sensitivity of Eq. 16 calculating $K(\theta)$ as unknown variable. In fact, despite the large difference between the estimation of $D(\theta)$ with VG-M (retention and diffusivity data) and VG-M (retention only) curve by Eq. 15, the influence of the specific water capacity $C(h)$, being the first derivative of the $\theta(h)$ curve, results in a much narrow gap between the respective $K(\theta)$ curves. In fact, except for the VG-M (retention only) model applied to Pure Pumice, which leads to a remarkable discrepancy in the wet range, the estimated functions are close to each other, relatively to each substrate. In this respect, the RETC code computation of experimental data coming only from One-Step procedure provides a sound basis comparison with the improved iterative method by Bibbiani (2002).

Conclusions

This study aims to compare different methods for the simultaneous determination of the hydraulic properties of growing media from One-Step experiment, exploiting the capability of the latter procedure to estimate the diffusivity function. Valiantzas *et al*. (1988, 1990, 2007) and Valiantzas and Londra (2012) set up attractive equations for this task. From their approach stems the Bibbiani (2002) improvement of the estimation method, based on Brooks and Corey equation for water retention, and Kozeny power equation for hydraulic conductivity. An independent set of 9 water retention experimental data allows the comparison of estimated curves. Moreover, the RETC software with the Van Genuchten model is performed, resulting in other two estimations of the hydraulic function: the first one coming only from water retention experimental data, the second one computing retention and diffusivity

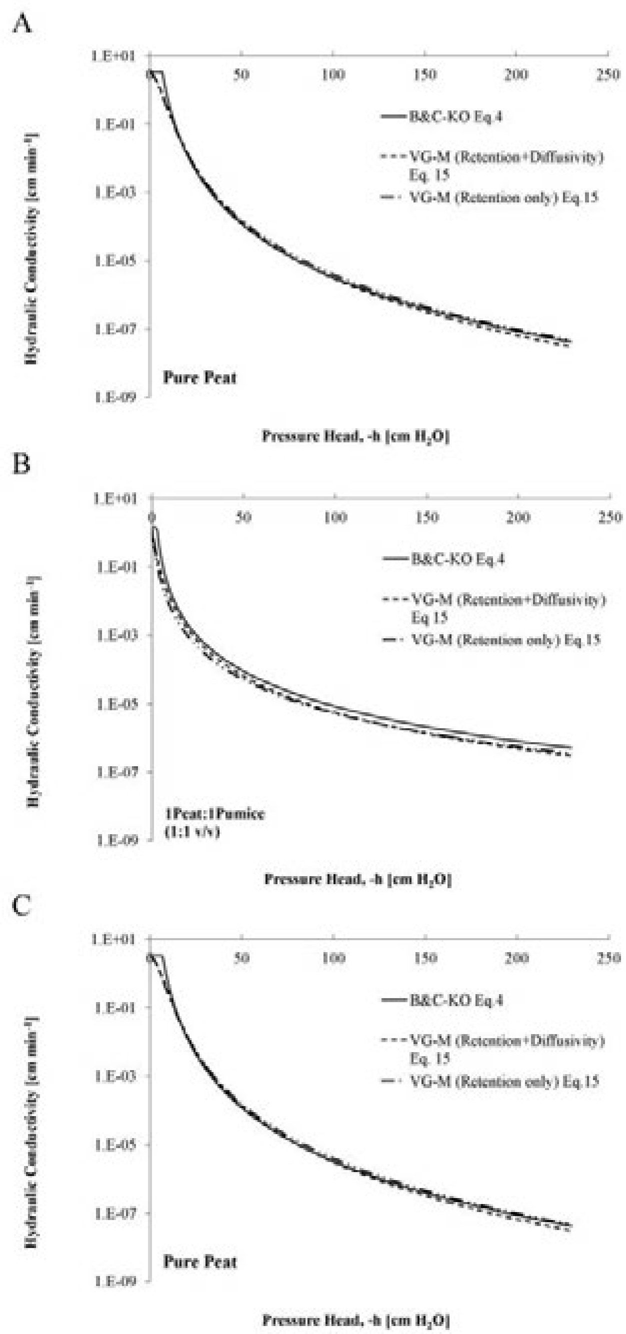

Figure 3. Substrate water conductivity K(h) as a function of pressure head -h, estimated by various equations. (A). Pure Pumice (B). 1Peat:1Pumice (1:1 v/v) (C). Pure Peat.

data from One-Step experiment.

Due to different requirements related to the final pressure head applied in One-Step experiment, Bibbiani's method leads to a good estimation of hydraulic functions for the three horticultural substrates in agreement with the Van Genuchten model, while the Valiantzas and Londra (2012) set of equations show poor applicability to this particular choice of the final pressure head.

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