

Determination of the water diffusivity of horticultural substrates: comparison of different approaches for the one-step outflow data analysis

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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, was performed on pure peat, pure pumice, and peat/pumice (1peat:1pumice by volume) mix, and compared with simplified equations by Valiantzas and Londra, who set up a new two-point method for calculating the water diffusivity, and with Van Genuchten-Mualem model. Brooks and Corey equations for water retention and hydraulic conductivity characterized the hydraulic properties of the porous media in relation to the iterative procedure. In the present work, the estimated water retention curves are compared with nine experimental data, and with the estimation of the Van Genuchten-Mualem model, via the RETC code, taking into account retention and diffusivity data. Bibbiani's and Van Genuchten-Mualem's estimations overlap except for the *very wet* range near saturation (R^2 equals to 0.9997, 0.9999, 0.9998 for pure pumice, 1peat:1pumice mix, and pure peat respectively, for Bibbiani's estimation; R^2 equals to 0.9923, 0.9541, 0.9993 for pure pumice, 1peat:1pumice mix, and pure peat respectively, for Van Genuchten-Mualem's estimation), whereas the Valiantzas and Londra's procedure didn't get satisfactory results, apparently because of different requirements related to the final pressure head applied in one-step experiment. In regard to diffusivity, a good similarity between Bibbiani's and Van Genuchten-Mualem's curves can be assessed, being the mean ratio values of the $D(\theta)$ from Valiantzas equation divided by $D(\theta)$ from Bibbiani equation equal to 1.20, 1.10,

and 1.31 for pure pumice, 1peat:1pumice mix, and pure peat respectively, 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.

Introduction

Water flow and solute transport modelling must rely on the knowledge of water retention and hydraulic conductivity curves, namely $\theta(h)$ and $K(\theta)$ 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 that could predict $K(\theta)$ from the moisture retention curve coupled by K_s 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 $D(\theta)$ relationship with one-step outflow data, being diffusivity the ratio of conductivity to the specific water capacity $C(h)=dq/dh$. 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 $D(\theta)$ employing equations from Valiantzas (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 $\theta(h)$ and $K(h)$ curves, leads to the estimation of the hydraulic characteristics, as well as the Van Genuchten-Mualem model.

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 packing procedure described by Bibbiani (2002), the substrate samples were subjected to the one-step procedure. An initial pressure equal to -1 kPa referred to the core centre was applied; once equilibrium was reached, a sudden application of a positive gas pressure increment marked the

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Contributions: the authors contributed equally.

Key words: hydraulic characteristics of substrates, one-step experiment, parameter estimation.

Received for publication: 25 October 2013.

Accepted for publication: 7 January 2014.

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Journal of Agricultural Engineering 2013; XLIV:219

doi:10.4081/jae.2013.219

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initiation of the outflow process recorded with time until equilibrium at the new pressure. Final pressure at -10 kPa has been chosen as the most suitable (Bibbiani, 2002). A duration of 48 h proved to be sufficient to allow for the necessary equilibrium and calculations. The above samples were re-saturated and a drying retention curve determined, along with other hydraulic parameters such as saturated hydraulic conductivity K_s , total porosity θ_{TP} , free-drainage water content θ_{fd} .

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

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

where $q = d\theta/dt$ 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 $D(\theta)$. Bibbiani (2002), in order to remove the limitation due to the absence of the θ_r parameter, re-introduced the latter in the relative water content Θ equation. Thus, the proposed equations are written as: i) Brooks and Corey's (B&C, as referred herein after), for water retention

$$\Theta = \left[\frac{He}{h} \right]^\lambda \quad h > He \quad (2)$$

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = 1 \quad 0 \leq h \leq He \quad (3)$$

ii) and for conductivity

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

where θ_s is the saturated water content, θ_r is the residual water content, He is the air-entry value, p and λ are fitting parameters (see Table 1 for units).

Eq. (2), (3), and (4) can be substituted for $D(\Theta)$ equation obtaining:

$$D(\Theta) = B \cdot (\Theta)^A \quad (5)$$

Table 1. List of symbols.

Variable	Description	Units	Variable	Description	Units
θ_{TP}	Total porosity	m^3m^{-3}	λ, p	Eq. (2), (4) B&C parameters	-
θ_s	Saturated water content	m^3m^{-3}	L	Core height	m
θ_{fd}	Free-drainage water content	m^3m^{-3}	He	Air-entry value	m
θ_i	Initial water content	m^3m^{-3}	A, B	Eq. (9) parameters	-
θ_f	Final water content	m^3m^{-3}	F, G	Eq. (12) V&L parameters	-
θ_r	Residual water content	m^3m^{-3}	α, m, n	Eq. (13), (15) VG-M parameters	-
θ_y	Water content at h_y matric potential	m^3m^{-3}	K_s	Saturated hydraulic conductivity	ms^{-1}
h	Matric potential	Pa	$Kr(\Theta)$	Relative hydraulic conductivity	-

B&C, Brooks and Corey; V&L, Valiantzas and Londra; VG-M, Van Genuchten-Mualem.

$$B = \frac{K_s He}{\lambda (\theta_s - \theta_r)} \quad (6)$$

$$A = p - 1 - \frac{1}{\lambda} \quad (7)$$

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

$$\theta_s = \frac{3\theta_{TP} + \theta_{fd}}{4} \quad (8)$$

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

$$q(\theta) = \frac{B \lambda^*(\mu)}{(A+1) L^2 (\theta_s - \theta_r)^A} \cdot [(\theta_i(\mu) - \theta_r)^{A+1} - (\theta_f - \theta_r)^{A+1}] \quad (9)$$

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

$$S(\theta_r, \lambda) = \sum_{y=1}^M \left\{ \ln \left[\frac{\theta_y - \theta_r}{\theta_s - \theta_r} \right] - \lambda \cdot \ln \left[\frac{\lambda (\theta_s - \theta_r)}{K_s} B_{(\omega_c)} + \lambda \cdot \ln [h_y] \right] \right\}^2 \quad (10)$$

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

Thus, the minimum value function $S(\theta_r, \lambda)$ can be plotted, and its minimum singles out the best fitting vector $[\theta_r, \lambda]$. Eq. (6) and (7) give parameters He and p , and so functions $\theta(h)$ 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 $D(\theta)$ analysing only the part of the curve where the cumulative outflow V ceases to be linear with respect to the square root of time \sqrt{t} . Later on, Valiantzas *et al.* (2007) and Valiantzas and Londra (2012) (V&L, as

referred herein after) 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:

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

which is related to cumulative outflow V vs the square root of time \sqrt{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 V&L equation:

$$D(\theta) = -\frac{2 \cdot (G-1) \cdot L^2 \cdot F^2 / G}{\pi^2} \left(\frac{\theta - \theta_f}{\theta_i - \theta_f} \right)^{-2/G} \quad (12)$$

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 θ_s from Eq. (8). The fitting program RETC (Van Genuchten *et al.*, 1991) estimated θ_r , α , and n unknown parameters, computing both experimental retention data coming only from one-step experiment and diffusivity data calculated by Eq. (5).

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

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

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

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

Finally, RETC code estimated the diffusivity $D(\theta)$ taking as input only 9 experimental moisture retention data, and the other hydraulic functions as well, thus resulting in the VG-M (retention only) curves.

Results and discussion

Table 1 shows the list of symbols applied in equations and units. Table 2 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 3 shows the estimated parameters for Eq. (2) and (5), as related to the B&C model improved by Bibbiani (2002).

Table 4 refers to Eq. (12), giving parameters of the new dimension-

less 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, $D(\theta)$, can be carried on applying the estimated parameters (Table 3 and Table 4) to the above discussed equations, and plotting the so-calculated curves, as shown in Figure 1. Irrespective to the substrate nature, there

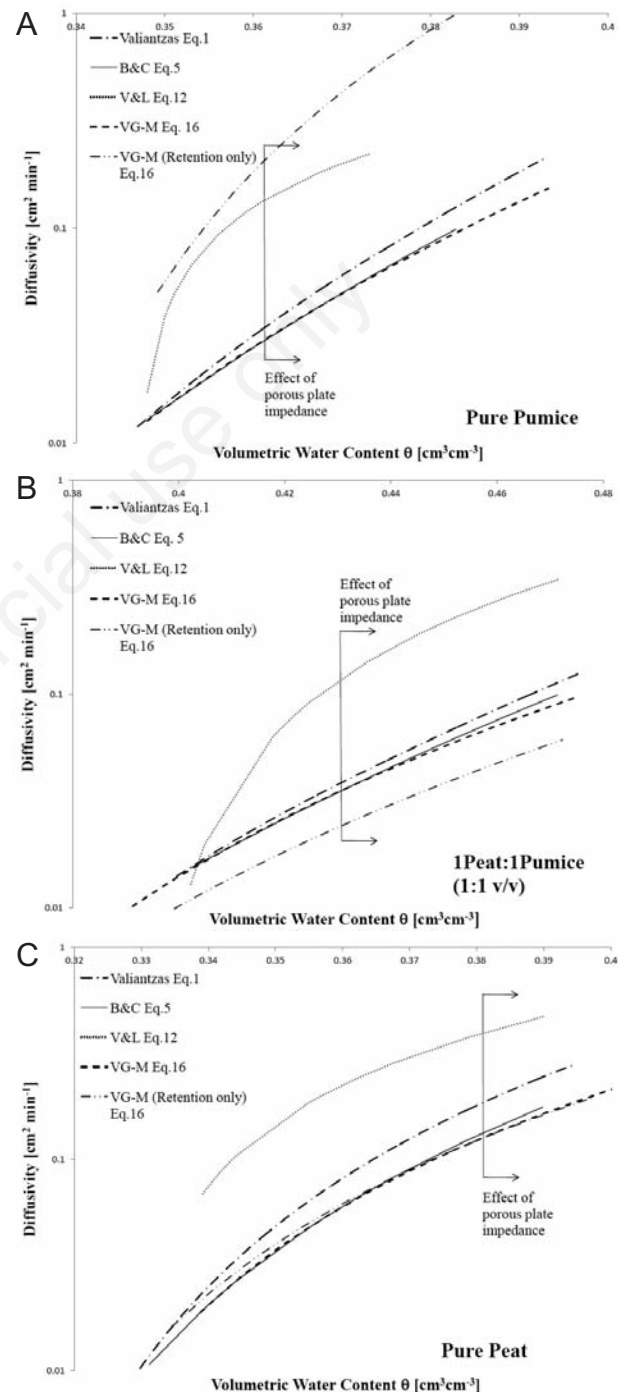


Figure 1. Substrate water diffusivity as a function of volumetric water content, $D(\theta)$, estimated by different equations. A) Pure pumice; B) 1peat:1pumice (1:1 v/v); C) pure peat. The short vertical line labeled *Effect of the porous plate impedance* defines the region where the plate impedance is not negligible.

is a good agreement between the direct calculation of $D(\theta)$ from Eq. (1), and both the B&C model by Eq. (5) and the VG-M model from Eq. (16) (retention and diffusivity data), being the mean ratio values of the $D(\theta)$ from Eq. (1) divided by $D(\theta)$ from Eq. (5) equal to 1.20, 1.10, and 1.31 for pure pumice, 1peat:1pumice mix, and pure peat respectively. VG-M model by Eq. (16) shows similar mean ratio values.

In contrast, the VG-M (retention only) curve shows a variable and unpredictable behaviour, suggesting a non-reliable estimation based only on retention data, being the mean ratio values of the $D(\theta)$ from Eq. (1) divided by $D(\theta)$ from Eq. (16) (retention only) equal to 2.10, 0.95, and 1.29 for pure pumice, 1peat:1pumice mix, and pure peat respectively. No explanation of the different performance of this model

Table 2. Water retention data sets and one-step pressure heads set-up.

Pure peat Pressure Head h [hPa]	Water Content θ [m ³ m ⁻³]	1peat:1pumice Pressure Head h [hPa]	Water Content θ [m ³ m ⁻³]	Pure pumice Pressure Head h [hPa]	Water Content θ [m ³ m ⁻³]
3.8=' θ_{id} '	0.879	3.8=' θ_{id} '	0.729	3.8=' θ_{id} '	0.465
10=' θ_i '	0.713	14=' θ_i '	0.574	10=' θ_i '	0.393
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=' θ_i '	0.329	104=' θ_i '	0.395	100=' θ_i '	0.347
140	0.318	147	0.376	140	0.340
230	0.309	233	0.361	230	0.335

Table 3. Measures parameters at saturation, and parameter estimation obtained for Eq. (2), (3), (4), (5), (6) and (7). B&C model.

Substrate	ρ kg m ⁻³	θ_{TP} m ³ m ⁻³	θ_s m ³ m ⁻³	Ks cm min ⁻¹	$\bar{\theta}_r$ m ³ m ⁻³	A($\bar{\theta}_r, \bar{\lambda}$) -	B($\bar{\theta}_r, \bar{\lambda}$) -	$\bar{\lambda}$ -
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

R² values equal to 0.9998, 0.9999, 0.9997 for pure peat, peat/pumice (1Pe:1Pu) mix, and pure pumice respectively.

Table 4. 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) Van Genuchten-Mualem VG-M (retention only) model. Simultaneous fit of retention and diffusivity data from one-step experiment for Eq. (13) VG-M model.

Variable	Pure peat Value	St.dev.	1peat:1pumice Value	SD	Pure pumice 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)						
θ_r	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	
R ²	0.9993		0.9995		0.9964	
Simultaneous fit of retention and diffusivity data from one-step experiment. 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	

SD, standard deviation.

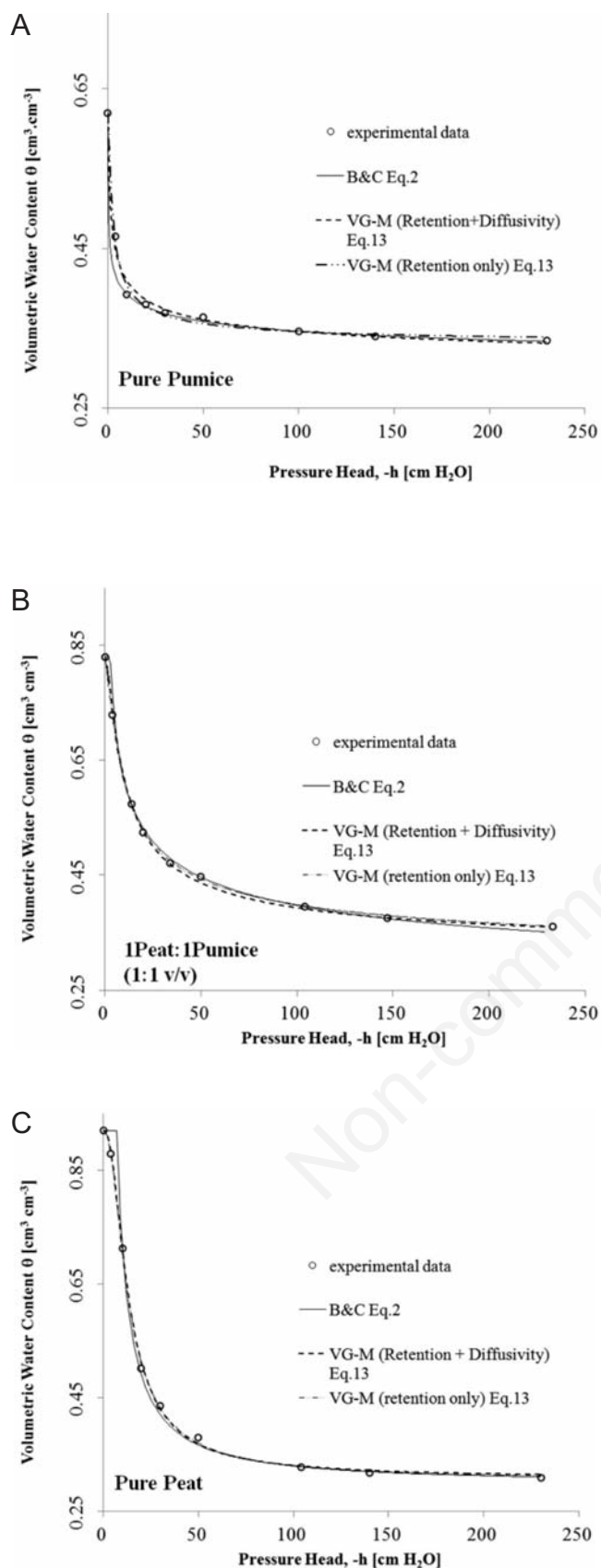


Figure 2. Substrate water retention $\theta(h)$ as a function of pressure head $-h$, measured and estimated by B&C and VG-M equations. A) Pure pumice; B) 1peat:1pumice (1:1 v/v); C) pure peat.

with the different characteristics of the substrates was found.

The prediction of $D(\theta)$ by Eq. (12) doesn't match any other ones in this experiment, being the mean ratio values of the $D(\theta)$ from Eq. (12) divided by $D(\theta)$ from Eq. (1) equal to 0.63, 5.22, and 1.13 for pure pumice, 1peat:1pumice mix, and pure peat respectively. 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 $-14 \div 18$ kPa. Doing this way, they assumed that q_f is very close to the q_r value, thus letting the estimation of the first iterative value for θ_f^0 ; on the contrary, in this paper, the final pressure head $h(\theta_f)$ 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-M plot of the function, as well. As one can see, the main difference between B&C Eq. (2) and VG-M Eq. (13) estimated curves lies in the very wet range (*i.e.* $h(\theta) < -1$ kPa), being all the rest almost overlapped. The correlation coefficient R^2 equals to 0.9997, 0.9999, 0.9998 for pure pumice, 1peat:1pumice mix, and pure peat respectively, for B&C estimation; R^2 equals to 0.9923, 0.9541, 0.9993 for pure pumice, 1peat:1pumice mix, and pure peat respectively, for VG-M estimation. 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): the mean ratio values of the $K(\theta)$ from Eq. (4) divided by $K(\theta)$ from Eq. (16) (retention and diffusivity data) equal to 0.92, 1.52, and 1.11 for pure pumice, 1peat:1pumice mix, and pure peat respectively.

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, 2007), Valiantzas and Kerkides (1990) 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 equations for hydraulic functions. An independent set of 9-water retention experimental data allows the comparison of estimated curves. Moreover, the RETC software with the Van Genuchten-Mualem 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 reten-

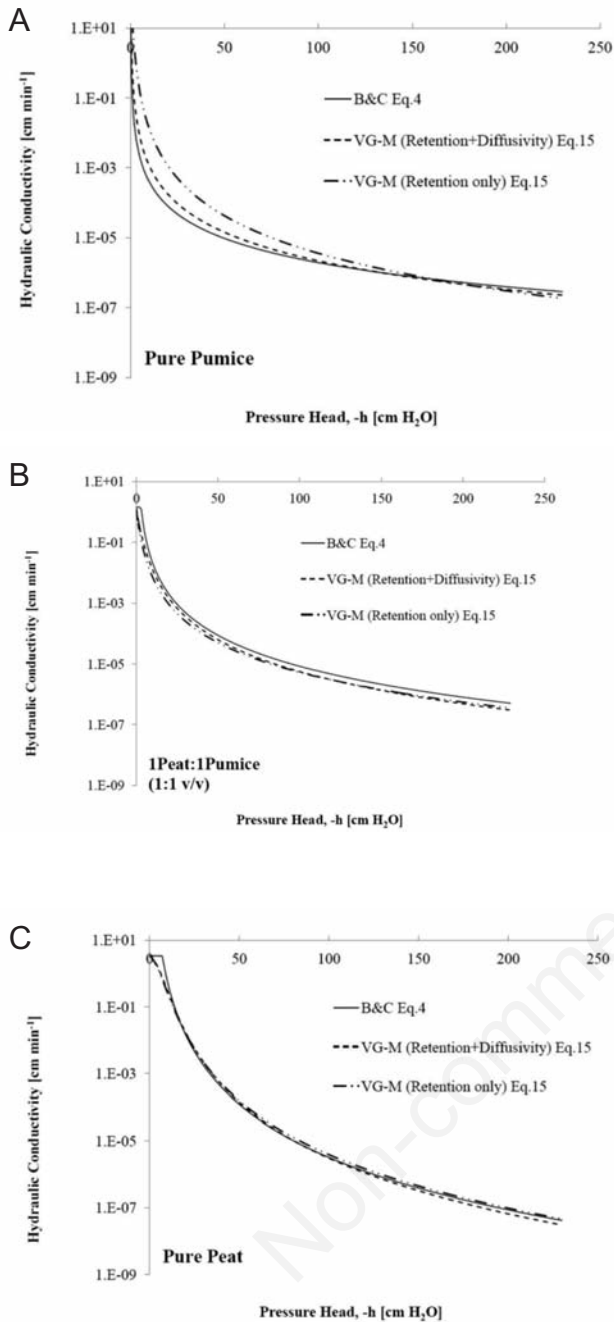


Figure 3. Substrate water conductivity $K(h)$ as a function of pressure head $-h$, estimated by different equations. A) Pure pumice; B) 1peat:1pumice (1:1 v/v); C) pure peat.

tion and diffusivity 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-Mualem model, while the Valiantzas and Londra (2012) set of equations shows poor applicability to this particular value of the final pressure head.

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