

Dear Editor,

We are very grateful to editor and reviewers for the constructive comments and suggestions on our manuscript (Manuscript ID: hess-2017-668). We have revised the manuscript according to these  
5 comments and now submit a point-by-point response, a marked manuscript and a revised manuscript.  
We hope the revised manuscript would meet with publication requests.

Looking forward to hearing from you

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Best regards,

Dong-hui Cheng

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### **A list of all relevant changes made in the manuscript**

- 5 1. Adding 7 soil samples with more clay content to validate the proposed model.
2. Comparing proposed model with the scaling approach proposed by Meskini-Vishkaee et al. (2014) and also adding the predicted results and discussions.
3. Adding a detailed transformation for Equation (4) in revised manuscript.
4. The discussions corresponding to the slit-shaped spaces have been added in our revised manuscript.
- 10 5. Revising the other small points suggested by reviewers.
6. Checking and correcting the minor mistakes in the text

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## A point-by-point response to reviewers and editor

### Reviewer 1 (F. Meskini-Vishkaee)

5 **1.** Since the relationship between the PSD and the pore size distribution (PoSD) is a fundamental element when predicting the SWRC from the PSD, first adjective of this study was to compare the estimated PoSD using traditional Method with the measured PoSD. The following comments and responding responses is about PoSD and PSD.

#### Comment a:

10 This step includes i, estimated PoSD from PSD and ii, estimated PoSD from SWCC. The authors have to change subtitle "2) measuring the PoSD" in page 3, line 33 by "2) estimating the PoSD from SWCC".

#### Response:

According to the Reviewer's suggestion, we have changed subtitle "(2) measuring the PoSD" in page 4, line 3 into "(2) estimating the PoSD from SWC".

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#### Comment b:

To estimate PoSD from PSD, called the traditional method as Arya model, here a proportionate relationship between pore size and associated particle diameter was used to calculate the equivalent pore diameter (Eqn. 2) because it was easy to use. This simplification may be a part of the estimation error of Arya and Paris (1891) model.

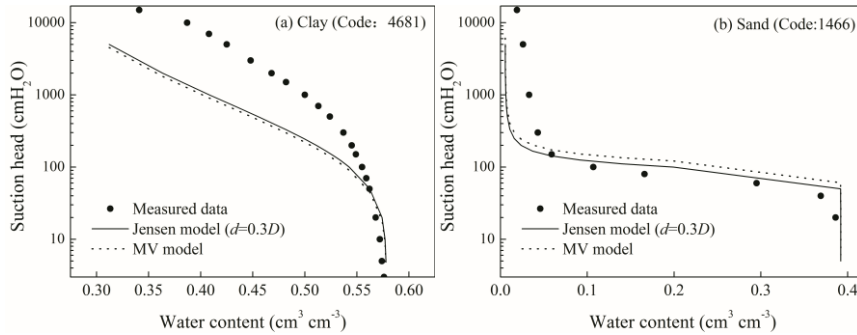
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#### Response:

The proportional relationship between the pore size and the associated particle size proposed by Jensen et al (2015) was used to calculate the equivalent pore diameter and the suction head in our manuscript. In order to evaluate the applicability of this method, we calculated the suction head using this proportional relationship and the water content followed the way of A&P model (Arya and Paris, 1981), and predicted the corresponding SWC, moreover compared them with the predicted SWCs using method in MV model (Mohammadi and Vanclooster, 2011) (Figure 1). We concluded that this proportional relationship proposed by Jensen et al. (2015) not only could get a good prediction of suction as the results calculated using the method in Mohammadi and Vanclooster (2011), also was easy to use.

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30 It should be noted that this calculation method of suction head was different from that in Arya and Paris (1891) model in which the pore diameters were estimated using the parameter  $\alpha$  to scale the pore length and pore volume.



**Figure 1: Measured SWC curves and predicted SWC curves using the methods proposed by Jensen et al (2015) and Mohammadi and Vanclooster (2011) respectively**

5 **Comment c:**

It is noted that estimation method of PoSD from SWCC is nearly similar to the estimation method of PoSD from PSD proposed by Mohammadi and Vanclooster (2010). Although, since SWCC is influenced both soil texture and structure, if soil organic carbon or clay content would be high, differences between estimated PoSD from SWCC and PSD become more. It must be mentioned that the prediction error of estimated SWCC from PSD is at dry range of SWCC (at high suction heads) that influences by soil texture (especially clay particles). Mohammadi and Meskini-Vishkaee (2012) attribute the methods error to the roughness of soil particles, high surface energy content of clay particles and the simplified pore geometric concepts that does not effectively reflect the pore geometry. It is better that the authors compare estimated PoSD from measured SWCC to estimated PoSD from PSD using similar method (use Mohammadi and vanclooster method as traditional method). Therefore, I think that these calculations have to add to this part of manuscript.

**Response:**

We agree with the reviewer's viewpoint that the error of predicted SWC from PSD in dry range (at high suction heads) that is influenced by soil texture (especially clay particles).

As mentioned in the comments, the estimation method of SWC from PSD is nearly similar to the estimation method proposed by Mohammadi and Vanclooster (2011). Mohammadi and Vanclooster (2011) calculated the suction head by assuming a linear relationship between the suction head and packing state, and the packing state is estimated from particle and bulk densities. Their suction head calculation method is given by

$$\psi_i = \frac{0.543 \times 10^{-4}}{R_i} \zeta \quad (1)$$

where  $\zeta$  is a coefficient depending on the state of soil particles packing;  $R_i$  is the particle radius. When calculating PoSD from SWC, a critical step is to estimate the pore size from the suction, but the calculation method of suction head in Mohammadi and Vanclouster (2011) (Eq.(1)) is the function related the suction head and the particle radius, not the relation of the suction head and the pore size. Therefore it could not be used for calculating PoSD from SWC.

2. Tuller et al. (1999) and Or and Tuller (1999) proposed including the water films coating the pore walls and water in angular spaces of pores, in calculations of soil water content. Despite great scientific interest, the proposed approach for the derivation of SMC by Or and Tuller (1999) motivated by bundle of cylindrical tubes limitations, usually fails to describe experimental data in the intermediate soil water content range because of the low flexibility of the gamma distribution function used to characterize the PoSD (Lebeau and Konrad, 2010). In addition, the model is mathematically complex and furthermore needs specific surface area parameter which measurements and estimations are often quite variable (Carter et al., 1986). The following two comments and responses are related to the pore geometry model and its parameters.

**Comment a:**

The authors use pore geometry containing slit-shaped spaces proposed by Or and Tuller (1999), But they assumed that circle-shaped central pore connected to two slit-shaped spaces. Moreover, the estimated PoSD data were fitted using a modified logistic growth model (Eqn. 5).

**Response:**

We go along with the reviewer's comments above. The pore geometry containing slit-shaped spaces proposed by Or and Tuller (1999) is regarded as a more realistic description for natural pore spaces. We used closely similar pore model which containing circle-shaped central pore connected to two slit-shaped spaces to predict SWC and could get the good fit with the measured SWC.

**Comment b:**

Specific surface area (SSA) is a requirement parameter to obtain the values of  $\alpha$  and  $\beta$ . The authors used a power equation with two fitting parameters (Eqn. 10) to estimate SSA proposed by Sepaskhah et al. (2010). Sepaskhah et al. (2010) used twenty soil samples from a depth of 0–30 cm were collected from different locations in Fars

province, in the south of Iran to calibrate the power equation. In addition, a different set of data was used to validate the calibrated model. Their results indicated that in the range of around 20 up to 200 m<sup>2</sup> g<sup>-1</sup> the values of measured SSA were in quite a good agreement, while for SSA greater than 200 m<sup>2</sup> g<sup>-1</sup>, the deviations increase distinctly. Moreover, Tuller and Or (2005) stated that the psychrometric approach for SSA determination should provide reliable values for natural soils with hydratable surface areas below 200 m<sup>2</sup> g<sup>-1</sup>. They recommend using SWCC values for -10 MPa and lower (drier) with an effective Hamaker constant of  $-6 \times 10^{-20}$  J to predict SSA values. So, there are some ambiguities here,

i. As respects higher SSA is related to finer texture soils that usually have underestimation problem of estimated SWCC from PSD, Indeed, I think use power model to estimate SSA cannot be useful to improve estimated SWCC in fine-textured soils. Page 9, line 4: the authors declared that "for the coarse-textured soil, the water content and prediction error of the SWCC changed relatively little for the same degree of change of the SSA". This is completely expected because not only there is not serious problem to estimate SWCC from PSD in coarse-textured soils, but also the value of estimated SSA using power equation is below 200 m<sup>2</sup> g<sup>-1</sup> for coarse-textured soils.

ii. Is there any SSA measurement? Were the fitting parameters of power model controlled?

**Response:**

(1) The response to the comment on the SSA estimation error

As reviewer mentioned above that the power function used to estimate the SSA are in quite a good agreement with the measured SSA when the values of measured SSA are in the range of around 20 up to 200 m<sup>2</sup> g<sup>-1</sup>, while for measured SSA greater than 200 m<sup>2</sup> g<sup>-1</sup>, the deviations increase distinctly (Sepaskhah et al., 2010). Moreover, their study showed that the power function with an  $r^2$  value of 0.88 is superior to the physical model and the multivariate pedo-transfer function for the estimation of SSA.

In our method, the values of parameter  $\alpha$  and  $\beta$  were firstly figured out using SSA and the measured SWC, and then these parameters were used for predicting SWC as input parameters. For the predicted SWCs of fine-textured soils which calculated from the parameter  $\alpha$  and  $\beta$ , the errors from estimated SSA, to some extent, could be offset by the parameter  $\alpha$  and  $\beta$ . Besides, the parameter  $\alpha$  and  $\beta$  were main used to estimate the volume fraction of the slit-shaped spaces, thus the estimation accurate of SSA influence the estimation of the volume fraction of the slit-shaped spaces, consequently the degree of improvement of predicted SWC. Overall there are always different levels of improvement comparing with the SWC predicted by the traditional method for all samples. Certainly, more effort should be directed to a more accurate method of SSA estimation.

We have added the discussions about the effect of the power equation to the SSA estimation in revised manuscript.

(2) The response to comments on the effect of SSA to the coarse-textured soil

As pointed out by reviewer, the factors that the water content and the prediction error of the SWC changed relatively little under the same proportional change of the SSA for coarse-textured soils include two aspects. We have enriched some discussions in Section 4.3.2 in our revised manuscript.

Meanwhile, although the absolute errors of predicted water content to measured water content using traditional models for fine-textured is higher than that for coarse-textured soil. However the relative errors of both fine-textured and coarse-textured soils cannot be ignored.

(3) The response to the comments on the SSA measurement

We regret that we do not conduct SSA measurement. The power equation employed to predict SSA in our manuscript is an empirical equation, and the parameters values in our manuscript cited Sepaskhah et al. (2010).

3. At the first step, the estimated PoSDs of 48 soil samples using SWRC were compared with the PoSDs calculated using PSD to identify the origins of the errors and their effects on the accuracy of the SWC and to calibrate the proposed model. Subsequently, 22 soil samples were also selected from UNSODA database to validate the model. The following three comments and responses are related to the data sets of the soil samples

**Comment a:**

Please provide a Table involved some properties of selected samples for both calibration and validation data sets (e.g. max, min and average of clay content, organic matter, bulk density and.....for each soil textural class).

**Response:**

The detailed information for both validation and calibration data sets are presented in Table 1 and Table 2, respectively.

**Table 1: Basic soil properties of 29 samples for the model validation.**

Soil texture	Number of soil		Clay (%)	Sand (%)	$\rho_b$ (g m <sup>-3</sup> )
Clay	5	Min	43	5.4	1.1
		Max	57	32	1.5
		Average	51	14.4	1.31
Loamy	2	Min	16.5	47.9	1.41
		Max	29.2	43.6	1.45

Loamy sand	5	Min	1.7	75.5	1.37
		Max	7.3	85.2	1.59
		Average	4.9	81	1.46
Sand	5	Min	1.1	90.1	1.46
		Max	4.4	97.5	1.58
		Average	2.3	93.4	1.53
Sandy loam	2	Min	11.4	56.8	1.44
		Max	12.6	65.7	1.46
Sandy clay loam	6	Min	9.8	28	1.21
		Max	30.7	69.7	1.53
		Average	22.8	43.2	1.45
Clay loam	4	Min	33.4	20.4	1.07
		Max	37.5	34.7	1.58
		Average	35.1	24.8	1.27

**Table 2: Basic soil properties of 48 samples for the model calibration.**

Soil texture	Number of soil		Clay (%)	Sand (%)	$\rho_b$ (g m <sup>-3</sup> )
Clay	9	Min	41.5	6.1	1.08
		Max	58.2	36	1.64
		Average	50.2	14.1	1.29
Loam	4	Min	14	42	1.36
		Max	23	67	1.63
		Average	17.3	50.5	1.46
Loamy sand	10	Min	3	76.2	1.32
		Max	10.4	89.4	1.6
		Average	6.1	83.2	1.46
Sand	16	Min	0.7	89.6	1.41
		Max	4.6	98.9	1.7
		Average	2.5	93.4	1.55
Sandy clay loam	1		2.7	62.5	1.7
Sandy loam	3	Min	10.5	64.9	1.27
		Max	19.4	76.3	1.7



		Average	15	68.8	1.50
Silt loam	5	Min	10.5	21	1.49
		Max	15.7	34.8	1.56
		Average	12.6	26.5	1.52

**Comment b:**

About validation data set, Textural distribution of the 22 soil samples is shown in both Figure 5 and Table 3. This duplication is not necessary.

5 **Response:**

Figure 5 in manuscript has been deleted in order to avoid repetition.

**Comment c:**

10 As regards the most prediction error of traditional models is often related to soils with good structure or high clay content. Therefore, the authors have to use more fine-textured soils to validate their proposed model. In validation data set, only 4 soil samples had clay texture and more than 60 % of soil samples are coarse-textured soils. Please add more soil samples with higher clay content and organic matter to the validation data set.

**Response:**

We have added 7 soil samples with clay content larger than 20% in order to fully validate the predicted model.

15 The added soil samples were summarized in Table 3.

**Table 3: Codes and textural classes of the added 7 soils selected from UNSODA**

UNSODA codes	Textual class
1320	Clay
1102, 2341	Sandy clay loam
3031, 3032, 1372, 1362	Clay loam

We have predicted the SWCs using the improved method, the scaling approach and the traditional method for the added soil samples respectively, and their predicted results and discussion have been added in revised manuscript.

4. The following comment is related to the calibration and validation of proposed model.

20 **Comment:**

In page 8, line 19-21: the authors stated that "These improvements are mainly attributed to the pore model containing slit-shaped spaces, demonstrating that this pore model is better for predicting the SWC from the PSD than the concept of a bundle of cylindrical tubes". This simplification (concept of a bundle of cylindrical tubes) is introduces as major source of error in the SWCC predictor models using PSD. After that, some studies have

attempted to improve the water content calculation approach by attributing model errors to both a simplified pore geometry and an incomplete desorption of residual water in the soil pore within the high matric suction head range. Therefore, I think the authors have to compare proposed model to other models except Arya and Paris (1981), such as Mohammadi and Meskini-Vishkaee (2012) or Meskini-Vishkaee et al. (2014) or other models.

- 5 The comparison between the performance of these models and parameter needs can be more helpful. Please expand discussion part and state the result of proposed model for both data sets (calibration and validation) in more detail.

**Response:**

- 10 We agree that quality of our manuscript will improve if the performances comparison between the proposed model and other improved models are added. Thus, we have compared our model with a scaling approach proposed by Meskini-Vishkaee et al. (2014) and added the predicted results and discussions in Section 4.2 in revised manuscript. (The estimation of SWCs for validation data are listed in Fig.S3 in the supporting information).
- 15 The results illustrated that the improved method here applied well to a wide range of soils, while the scaling approach performed better for fine- and medium-textured soils. The  $E_{\text{RMS}}$  values range from 0.017 to 0.054 for the improved method (with an average of 0.028), from 0.026 to 0.060 for the scaling approach (with an average of 0.037) and from 0.040 to 0.106 for the traditional method (with an average of 0.061). Among the three methods mentioned above, the improved method provided the best predictions and the traditional method
- 20 performed worst.

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## Reviewer 2

**Comment 1:** Detailed comments Equation (4) should be rewritten in a more general way, regardless of the units adopted for the water potential. In this regard, it seems that this equation is used to link pore dimension to water potential, even in the silt-shaped space between pores. This aspect should be better clarified, as the dimension of the silts are proportional to the pore diameter, so it is not clear what is the diameter introduced in equation (4) to obtain the corresponding potential.

### Response to comment 1:

(1) The transformation process of Equation (4) in the main manuscript

- 10 Equation (4) in our main manuscript was gained by substituting known parameters into Laplace's equation (Eq. (2))(Haverkamp et al., 1986), in which  $\sigma=7.275 \times 10^{-2} \text{ kg s}^{-2}$ ,  $\rho_w=998.9 \text{ kg m}^{-3}$ ,  $g=9.81 \text{ m s}^{-2}$ , and  $\varepsilon=0^\circ$  (Mohammadi and Vanclooster, 2011).

$$\psi_i = \frac{2\sigma \cos \varepsilon}{r_i g \rho_w} \quad (2)$$

- 15 Then, transforming  $r_i$  to  $d_i$  and the units to gain Eq. (3) (Eq. (4) in our main manuscript), which is more clear to express the relation between the pore diameter and suction head.

$$\psi_i = \frac{3000}{d_i} \quad (3)$$

We have added the transformation process above in our revised manuscript.

(2) The suction head calculation for slit-shaped spaces

- 20 Because the shape and size of slit spaces were different from the central pore, their suction heads were calculated using different equations respectively. The suction heads of central pore were calculated using Eq. (3), while the chemical potentials of slit spaces were calculated using Eq. (4) suggested by Derjaguin and Churaev (1992) and then transforming the units to gain the suction heads.

$$\mu = -2\sigma / (\rho \alpha d) \quad (4)$$

Where,  $\alpha$  is the scaling parameter of the slit width.

- 25 This aspect have been rewrote in Section 3.1 "Estimating the pore volume fraction" in the revised manuscript.

**Comment 2:** There is also another point, regarding silt-shaped spaces, that in my opinion deserves to be discussed in the paper. To my best understanding, silt-shaped spaces are introduced to consider the water which

is bonded to the particles in such a way that the model of the bundle of cylinders fails in describing it. In fact, with such silts dimensions as small as  $1 \text{ \AA}$  are reached. In such a range of dimensions, capillarity is not anymore the mechanism which bonds water to the soil particles, and other kinds of interactions contribute to the potential energy of water (actually, already for quite larger pore dimensions). So, if equation (4) is still used, this turns out to be an effective, but not physically based, way to obtain water potential.

**Response to comment 2:**

Nitao and Bear (1996) pointed out that the vague definition of the soil matric potential where capillary and adsorptive forces are lumped together. During drainage, when considering the capillary forces only, the drainage potential in slit-shaped pore is given as Eq.(7) (Derjaguin and Churaev, 1992) in revised manuscript, while the applicability of this formula is limited by condition the width of the slit. When passing over to thin slits, a correction will have to be introduced, taking into account the effect of adsorption force at the slit surfaces. Tuller and Or (2001) defined a critical slit spacing ( $ad^*$ ) by Eq.(16) in revised manuscript that would classify slit sizes responding to capillary drainage and adsorption dominated drainage. In case of slit spacing greater than  $ad^*$ , the capillary-based slit snap-off would be applied. The value of  $ad^*$  is 0.591 nm, it means that for slit spacing greater than 0.591 nm, the Eq.(7) could be applied to calculate the drainage potential in slit-shaped pore in revised manuscript.

Besides, a simplification was made in our study that we only take the water in central pore and slit spaces into account, without considering the liquid films coat pore and slit walls; therefore the capillary pressure, as the dominant acting forces, was only considered. Furthermore because the predicted suction head in our study is lower than  $5000 \text{ cmH}_2\text{O}$ , the error resulted from the lack of consideration of adsorptive surface forces were relative small. We have added a chapter to discuss the property of the slit-shaped spaces in the revised manuscript.

**Comment 3:** Pag. 5, line 13. The water potential values should be negative.

**Response to comment 3:**

Indeed, it's true that the critical potential values of the biggest slit spaces should be negative on Page 5, line 13. In order to compare in unified standard, this potential values were transformed into the suction head with unit of  $\text{cmH}_2\text{O}$ . It was our oversights that it not be described clearly; hence we have changed "critical potential" as "critical suction head" on Page 5, line 12 in revised manuscript.

**Comment 4:** Pag. 9, lines 17-19. This statement sounds surprising, if I understand it correctly. The smaller the particles, the larger I expect soil (specific) surface area, as for instance for clay particles. In this respect, the authors should try (where possible), or at least mention the possibility of using measured surface areas rather than estimating it by means of an empirical formula, and discuss how their results could be (positively or negatively) affected.

**Response to comment 4:**

The surface area ( $m^2$ ) on Page 9, lines 17-19 refer to the surface area of particle which is positively related to the equivalent particle radius and is different from the specific surface area ( $m^2 g^{-1}$ ) which is the total surface area of a material per unit of mass.

As reviewer mentioned that the deviations will generate when estimate the SSA using the power function. Moreover, their study showed that the  $r^2$  between the SSA predicted by the power function and the measured SSA is 0.88, it proved that this empirical equation have reliable capabilities to use.

Furthermore, the measured SSAs for so many samples were difficult for us at present. Therefore calculating the specific surface area using an empirical formula may be the best choice.

**Comment 5:** Pag. 10, line 21. The reference should read “van Genuchten, M. T.” instead of “Genuchten, M. T. V.”, and the same holds for where such a reference is recalled in the text.

**Response to comment 5:** Thank reviewer for pointing out our mistake. “Genuchten, M. T. V.” on Page 10, line 21 have changed into “van Genuchten, M. T.”.

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# Predicting the soil water characteristic curve from the particle size distribution based on a pore space geometry containing slit-shaped spaces

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10 **Abstract.** Traditional models employed to predict the soil water characteristic curve (SWC) from the particle size distribution (PSD) always underestimate the water content in the dry range of the SWC. Using the measured physical parameters of 48 soil samples from the UNSODA unsaturated soil hydraulic property database, these errors were proven to originate from the ~~inaccurate estimation of the pore size distribution, underestimation of the pore volume fraction of the minimum pore diameter range~~. A method was therefore proposed to improve the estimation of the water content in the high suction range using a pore model comprising a circle-shaped central pore connected to slit-shaped spaces; in this model, 15 pore volume fraction of the minimum pore diameter range and the corresponding water content were accordingly increased. The SWCs predicted using the improved method reasonably approximated the measured SWCs, and which were more accurate than those obtained using traditional method ~~and the scaling approach~~ in the dry range of the SWC.

## 1 Introduction

20 The soil water characteristic curve (SWC), which represents the relationship between the water pressure and water content, is fundamental to researching water flow and chemical transport in unsaturated media (Pollacco et al., 2017). Direct measurements of the SWC consume both time and money (Arya and Paris, 1981; Mohammadi and Vanclouster, 2011), while estimating the SWC from the particle size distribution (PSD) is both rapid and economical. Therefore, a number of associated conceptual and physical models have been proposed.

25 The first attempt to directly translate a PSD into an SWC was performed by (Arya and Paris, 1981) (hereinafter referred to as the AP model). In this model, the PSD is divided into multiple size fractions and the bulk and particle densities of the natural-structure sample are uniformly applied to each particle size fraction, from which it follows that the relative pore fraction and the relative solid fraction are equal. Thus, the degree of saturation can be set equal to the cumulative PSD function. The soil suction head can be obtained using the capillary equation based on a "bundle of cylindrical tubes" model, and the pore size in the equation is determined by scaling the pore length and pore volume (Arya et al., 2008). Based on the 30 principle of the AP model, many researchers have focused on improving the suction head calculations, which are commonly

based on the capillary equation; however, various methods are used to translate the particle diameter into the pore diameter (Haverkamp et al., 1986; Zhuang et al., 2001; Mohammadi and Vancloster, 2011; Jensen et al., 2015). Some models estimate the pore diameter based on particle packing patterns (e.g., the MV model), while others utilize the proportionality factor between the pore size and the associated particle diameter (e.g., the HP model and two-stage approach). However, the scheme employed to estimate the water content has not been modified and follows the approach of the AP model. The SWC predicting models which have the same scheme to predict the water content and only improve the suction head calculation are termed as the traditional models in following text.

However, these traditional models ~~which follow the water content calculation approach of the AP model~~ underestimate the water content in the dry range of the SWC (HwangSang and Powers, 2003; Meskini-Vishkaee et al., 2014). Therefore, some researchers have attempted to improve the water content calculation approach by attributing model errors to both a simplified pore geometry and an incomplete desorption of residual water in the soil pore within the high matric suction head range (Tuller et al., 1999; Mohammadi and Meskini-Vishkaee, 2012). Recent findings revealed the existence of corner water, lens water and film water in soils at high matric suction head (Tuller et al., 1999; Mohammadi and Meskini-Vishkaee, 2012; Or and Tuller, 1999; Shahraneeni and Or, 2010; Tuller and Or, 2005). Therefore, ~~(Mohammadi and Meskini-Vishkaee, (2012) predicted the SWC based on the PSD while considering adsorbed water film and lens water between the soil particles, and slightly improved upon the traditional MV model, and predicted the SWC based on the PSD while considering adsorbed water film and lens water between the soil particles.~~ (Tuller et al., (1999) proposed a pore space geometry containing slit-shaped spaces and derived a corresponding SWC that considered water film and water in angular-shaped pores; however, the SWC failed to describe experimental data at an intermediate water content due to the limitations of the gamma distribution function used to characterize the pore size distribution (PoSD) (Lebeau and Konrad, 2010). Moreover, this model was mathematically complex. (Mohammadi and Meskini-Vishkaee, 2013) incorporated the residual water content into the MV model and consequently decreased the magnitude of the underestimation in the dry range of the SWC. However, an accurate estimation of the residual water content remains a challenge. Meskini-Vishkaee et al (2014) improved the traditional MV model by defining a soil particle packing scaling factor, and this method could improve the estimation of the SWC, particularly significant for the fine- and medium-textured soils,

Many traditional models are based on a “bundle of cylindrical tubes” representation of the pore space geometry (Arya and Paris, 1981; Zhuang et al., 2001), which results in intrinsic errors when predicting water flow in variably saturated soils. Consequently, some researchers have considered pore networks as bundles of triangular tubes, which could incorporate the contribution of water in pore corners to the water content (Helland and Skjæveland, 2007). A new pore geometry model comprising a polygon-shaped central pore connected to slit-shaped spaces was proposed by Tuller et al. (1999) to provide a more realistic representation of natural pore spaces (Tuller et al., 1999; Or and Tuller, 1999; Tuller and Or, 2001). This pore model could represent a foundation for accurately describing the water status in natural soils, particularly in arid environments.

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The objectives of this study were therefore to evaluate the leading factors that lead to the underestimation of the water content in the dry range of the SWC using traditional methods and to furthermore propose a method for accurately estimating the water content using a pore space geometry containing slit-shaped spaces to improve the prediction of the SWC.

5

## 2 Basic descriptions

The relationship between the PSD and the PoSD is a fundamental element when predicting the SWC from the PSD. (HwangSang and Powers (2003) found that the nonlinear relationship between the PSD and the PoSD would be more appropriate than the linear relationship applied in the AP model and therefore described both the PSD and the PoSD as lognormal distributions. However, since the PSD and PoSD of soils do not strongly follow a lognormal distribution, this model performed very poorly for moderately fine-textured soils (Hwang and Choi, 2006). Obtaining an accurate PoSD from the PSD of a soil is highly difficult, and the errors that arise from this approach could cause inevitable errors in the SWC. However, the underestimation of the water content in the dry range of an SWC has not been comprehensively evaluated from this perspective.

15 In this study, the measured PoSDs of 48 soil samples were compared with the PoSDs (~~They were actually corresponding PSDs~~) calculated using a traditional model (~~they were actually corresponding PSDs~~) to identify the origins of the errors and their effects on the accuracy of ~~predicted~~the\_SWC. The provided 48 soil samples exhibited a wide range of physical properties (Table 1), and they were selected from the UNSODA unsaturated soil hydraulic property database, which contains 790 soil samples with general unsaturated soil hydraulic properties and basic soil properties (e.g., water retention, hydraulic conductivity, soil water diffusivity, PSD, bulk density, and organic matter content) (Nemes et al., 2001).

20 (1) Calculating the PoSD using a traditional model

Traditional models commonly assume that the pore volume fraction of each size fraction can be set equal to the relative solid fraction(Arya and Paris, 1981). Thus, the cumulative pore volume fraction can take the following form:

25

$$\sum_{j=1}^{j=i} v_i = \sum_{j=1}^{j=i} \omega_j; \quad i = 1, 2, 3, \dots, n$$

(1)

where  $\omega_j$  is the solid fraction of the  $j$ th particle fraction,  $v_j$  is the pore volume fraction associated with the  $j$ th fraction, and  $n$  is the total number of size fractions in the PSD.

The routine procedures employed among the several traditional models to translate a particle diameter into a pore diameter are different. The equivalent pore diameter can be derived from physical properties, including the bulk density and the particle density, or from the proportionate relationship between the pore size and associated particle diameter. Although

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the former can logically characterize a pore, a complicated pattern can slightly reduce the model performance.

While ~~Meanwhile~~, the latter approach is easy to use, and its rationality has been demonstrated by some researchers (Hamamoto et al., 2011; Sakaki et al., 2014). Here, the latter technique was applied, and it can be expressed as

$$d_i = 0.3D_i \quad (2)$$

5 where  $D_i$  is the mean particle diameter of the  $i$ th fraction ( $\mu\text{m}$ ),  $d_i$  is the corresponding equivalent pore diameter ( $\mu\text{m}$ ). Inputting the PSD data, then calculated pore diameters are sequentially paired with corresponding pore volume fractions to obtain a Calculated PoSD.

(2) Estimating the PoSD from SWC ~~Measuring the PoSD~~

It is generally difficult to measure the PoSD of a soil; however, the PoSD can be indirectly obtained using the measured water content and suction head (Jayakody et al., 2014). The cumulative pore volume fraction of the  $i$ th fraction is equal to the ratio of the measured water content to the saturated water content (Eq. (3)):

$$\theta_i = \theta_s \sum_{j=1}^{j=i} v_j; \quad i = 1, 2, \dots, n$$

~~$\theta_i = \theta_s \sum_{j=1}^{j=i} v_j; \quad i = 1, 2, 3, \dots, n$~~  (3)

where  $\theta_s$  is the saturated water content ( $\text{cm}^3 \text{cm}^{-3}$ ), and  $\theta_i$  is the measured water content ( $\text{cm}^3 \text{cm}^{-3}$ ).

15 Meanwhile, the corresponding pore diameters are derived on the basis of Laplace's equation capillary theory and Eq. (4).

$$\psi_i = \frac{3000}{d_i} \psi_i = \frac{2\sigma \cos \varepsilon}{r_i g \rho_w} \quad (4)$$

where  $\psi_i$  is suction head ( $\text{cmH}_2\text{O}$ ).  $\sigma$  is the surface tension ( $\text{kg s}^{-2}$ ),  $\varepsilon$  is the contact angle between the soil particle and water,  $r_i$  is the pore radius (m), and  $\rho_w$  is the density of water ( $\text{kg m}^{-3}$ ). Assuming for water at  $20^\circ\text{C}$ ,  $\sigma=7.275 \times 10^{-2} \text{ kg s}^{-2}$ ,  $\rho_w=998.9 \text{ kg m}^{-3}$ ,  $g=9.81 \text{ m s}^{-2}$ , and  $\varepsilon=0^\circ$  (Mohammadi and Vanclouster, 2011), then transforming  $r_i$  to  $d_i$  and substituting numerical values of the constants yields a simplified expression as Eq. (5).

$$\psi_i = \frac{3000}{d_i} \quad (5)$$

where  $\psi_i$  is suction head ( $\text{cmH}_2\text{O}$ ),  $d_i$  is the pore diameter ( $\mu\text{m}$ ). Then the pore diameter calculate by Eq. (5) were sequentially paired with cumulative pore volume fractions calculated by Eq. (3) to obtain a PoSD, which could be considered a measured PoSD.

25 ~~The PoSD obtained in this way is considered the measured PoSD.~~

The calculated and measured PoSD data were fitted using a modified logistic growth model (Eq. (6)) (Liu et al., 2003):

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$$w_i = \frac{1}{1 + a \exp(-bd_i^c)}$$

(65)

where  $w_i$  is the cumulative pore volume fraction with diameters smaller than  $d_i$  (%), and  $a$ ,  $b$ , and  $c$  are the fitting parameters (dimensionless). This model produced a good fit for the PoSD data employed in this study with a coefficient of determination ( $r^2$ ) that ranged from 0.972 to 0.999.

The measured pore volume fraction curves for the typical samples, namely, sand (code: 3172) and clay (code: 2360), and their calculated curves using the traditional model are presented in Fig. 1. The small maps embedded in Fig. 1 exhibit the measured and calculated PoSD curves. Figure 1 show that the calculated PoSD curves approximately coincide with the measured curves in the larger pore diameter range, while the calculated values in the smaller range, which correspond to the higher suction range on the SWC curve, are obviously smaller than the measured values. The underestimation of the pore volume fraction in the smaller pore diameter range can consequently lead to an underestimation of the water content at a higher suction range. In particular, the calculated pore volume fraction associated with the smallest pore diameter ( $d \leq 0.6 \mu\text{m}$ ) was far less than the measured pore fraction. These results illustrated that the underestimation of the pore volume fraction with respect to the smallest pore diameter ( $d \leq 0.6 \mu\text{m}$ ) was a key factor with regard to the underestimation of the water content in the dry range of the SWC. Besides, the underestimation of pore volume fraction is associated with an oversimplified pore space geometry, which traditional models have generally characterized as a bundle of cylindrical capillaries. The measured and calculated pore curves of the other 46 soil samples behaved in the same fashion, and those curves are provided in the supporting information (Fig. S1).

### 3 Improved method

#### 3.1 Estimating the pore volume fraction

In this study, the soil pore structure was conceptualized within a pore model in which the elementary unit cell is composed of a relatively larger circle-shaped central pore connected to two slit-shaped spaces (see Fig. 2). Relative to the polygonal central pore connected to slit-shaped spaces as described by Or and Tuller (1999), both the slit width and the slit length are proportional to the diameter of the associated central pore  $d$  and are therefore expressed as  $ad$  and  $\beta d$ , respectively.

When estimating the pore volume fraction using the pore model described above, the volume fractions of the central pore and slit-shaped spaces are distinguished. The slit-shaped pore spaces are accordingly classified into the smallest central pore size since the size of the slit-shaped pore spaces are smaller than the minimum central pore diameter. The particle sizes of our samples range from 2 to 2000  $\mu\text{m}$ , and the corresponding pore sizes are between 0.6 and 600  $\mu\text{m}$ ; meanwhile, the largest slit width calculated from the parameters in Table 2 is 0.24  $\mu\text{m}$ . In addition, when the drainage potential in slit-shaped pore is given as Eq.(7)  $\mu = 2\sigma/(\rho g d)$  based on the capillary theory (Derjaguin and Churaev, 1992),

$$\mu = \frac{-2\sigma}{\rho\alpha d} \quad (7)$$

where  $\mu$  is the critical potential (J kg<sup>-1</sup>), the critical potential for slit snap-off of the widest slit-shaped spaces, the critical suction head of slit snap-off is calculated using Eq.(7) is 6202 cmH<sub>2</sub>O (the potential is converted to the suction head),

which is smaller than the critical suction head/critical potential of 5000 cmH<sub>2</sub>O calculated using Eqs. (2) and (54) for the minimum central pore. This also demonstrates that the equivalent pore diameter of a slit space is smaller than the minimum central pore diameter. Therefore, the pore volume fractions of the soil samples were simplified into those of central pores, but the volume fractions of the minimum central pores contained the volume fractions of all slit-shaped spaces.

Coupled with the traditional assumption that the volume fraction of each unit cell (i.e., the central pore and two slit-shaped spaces) is equal to the relative particle mass fraction, using the geometric relationship described in Fig. 2, the volume fraction of central pore and slit-shaped spaces can be separated, then the pore volume fractions of different sizes can be readily obtained.

The procedure utilized to calculate the pore volume fraction is shown in Fig. 3. Assuming that the soil pores are composed of numerous unit cells with various sizes, the fraction of the  $i$ th unit cell is equal to the relative particle mass fraction  $\omega_i$ . The sum of the slit pore volume fractions of various sizes ( $\zeta_2 + \zeta_3 + \dots + \zeta_i$ ) and the volume fraction of the smallest unit cell ( $\omega_1$ ) form the volume fraction of the smallest pore ( $v_1$ ). Successively accumulating that volume fraction with the other central pore volume fractions (i.e.,  $v_2, v_3, v_4, \dots$ ) provides the PoSD of a sample. The slit pore volume fraction,  $\zeta_i$ , the volume fraction of the smallest pore  $v_1$  and the volume fractions of the other pores  $v_i$  were calculated using Eq. (86), Eq. (97) and Eq. (108), respectively:

$$\zeta_i = \omega_i \frac{2\alpha\beta d_i^2}{2\alpha\beta d_i^2 + \frac{\pi}{4} d_i^2}$$

(86)

$$v_1 = \omega_1 + \sum_2^n \zeta_i$$

(97)

$$v_i = \omega_i - \zeta_i$$

(108)

where  $\zeta_i$  is the slit pore volume fraction,  $v_i$  is the volume fraction of the  $i$ th pore fraction, and  $\alpha$  and  $\beta$  are the scaling parameters of the slit width and the slit length, respectively.

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### 3.2 Values of $\alpha$ and $\beta$

To obtain the values of  $\alpha$  and  $\beta$ , an expression containing both of these parameters with respect to the specific surface area ( $S_{SA}$ ) was applied here. The  $S_{SA}$  of the pore as shown in Fig. 2 can be described using a geometrical relationship as follows:

$$S_{SA} = \frac{\phi}{1000\rho_b} \sum_{j=1}^{i=j} \omega_i \frac{4\beta d_i + \pi d_i}{2\alpha\beta d_i^2 + \frac{\pi}{4} d_i^2}; \quad i = 1, 2, \dots, n$$

$$S_{SA} = \frac{\phi}{1000\rho_b} \sum_{i=1}^n \omega_i \frac{4\beta d_i + \pi d_i}{2\alpha\beta d_i^2 + \frac{\pi}{4} d_i^2}; \quad i = 1, 2, \dots, n$$

(119)

where  $S_{SA}$  is the specific surface area ( $\text{m}^2 \text{g}^{-1}$ ),  $d_i$  is the pore diameter (m),  $\rho_b$  is the bulk density ( $\text{kg m}^{-3}$ ) and  $\phi$  is the measured porosity. Therefore, an important requirement for the calculation of the  $\alpha$  and  $\beta$  values is an estimation of the sample-scale value of  $S_{SA}$ . Here, a power equation was applied as follows (Sepaskhah et al., 2010):

$$S_{SA} = 3.89d_g^{-0.905}$$

(120)

where  $S_{SA}$  is the estimated specific surface area ( $\text{m}^2 \text{g}^{-1}$ ), and  $d_g$  is the geometric mean particle size diameter (mm) obtained using Eq. (134) (Shirazi and Boersma, 1984):

$$d_g = \exp(f_c \ln M_c + f_{si} \ln M_{si} + f_{sa} \ln M_{sa})$$

(134)

where  $f_c$ ,  $f_{si}$  and  $f_{sa}$  are the clay, silt and sand fractions (%) of the soil sample, respectively,  $M_c$ ,  $M_{si}$  and  $M_{sa}$  are the mean diameters of clay, silt and sand that are empirically taken as 0.001 mm, 0.026 mm and 1.025 mm, respectively.

Consequently, the quantitative relationship between the parameters  $\alpha$  and  $\beta$  can be obtained using Eq. (119). Associated with the additional constraint of Eq. (120), the values of  $\alpha$  and  $\beta$  can be theoretically solved if the measured slit volume fraction or the measured SWC is known. However, an analytical solution is difficult to derive due to the high nonlinearity of both equations. Here, a trial and error approach was adopted that was much easier than the analytical method. Conveniently, UNSODA database provided a great deal of soil information, including measured SWCs and diverse physical properties.

The routine procedure for handling a soil sample involved the following steps. First, given the initial value of  $\alpha$ , the value of  $\beta$  was calculated using Eqs. (119)-(134), after which the PoSD was predicted using Eqs. (86)-(108). Subsequently, the SWC was estimated using the method described in Sect. 3.3. Finally, the value of  $\alpha$  was changed repeatedly until the newer predicted SWC was in good agreement with the measured SWC and the water content corresponding to a suction

head of 5000 cmH<sub>2</sub>O was within 90% of the measured data (see Fig.S2 in the supporting information). The results for the 48 soil samples indicated that the  $\beta$  values exhibited a broad range of variation for all samples, while the  $\alpha$  values showed regular changes with the soil texture. The relationship between the sand contents and  $\alpha$  values for the 48 samples is shown in Fig. 4, which clearly demonstrates that the values of  $\alpha$  are similar for samples with specific sand contents.

5 Therefore, the approach was simplified by setting  $\alpha$  as a constant for similar soil textures. The corresponding detailed descriptions are summarized in Table 2. The values of  $\alpha$  were in the range from 3.34E-05 to 2.12E-02, which were estimated by Or and Tuller (1999) using a pore-scale geometry model comprising a polygon-shaped central pore connected to slit-shaped spaces. According to the sand contents of the samples, Table 2 is a reference for determining the  $\alpha$  values that serve as input parameters in predicting the SWC from the PSD hereinafter.

### 10 3.3 Estimating the SWC

The values of  $\alpha$  and  $\beta$  for the various soil samples facilitated the acquisition of the volume fractions of the slit pores using Eq. (86) and the PoSD using Eqs. (97) and (108). The water contents associated with different pore filling stages could be estimated by substituting the PoSD into Eq. (3), and the pore size and the corresponding suction head could be calculated using Eqs. (2) and (54). The SWC could be ultimately obtained using the calculated suction heads and water contents.

## 15 4 Model validation

### 4.1 Data sources

~~Twenty-nine~~ ~~Twenty-two~~ soil samples with a wide range of physical properties were also selected from UNSODA database to validate the model; the codes ~~and contents~~ of the samples are summarized in Table 3 ~~and Fig. 5~~. For the soil samples that were not provided with a saturated water content  $\theta_s$ , the first data point of the measured SWC corresponding to the lowest suction head was regarded as  $\theta_s$ .

To generate a detailed PSD, a modified logistic growth model (Eq. (65)) was used to fit the measured PSD data. Here, the detailed PSD was generated at diameter classes of 2, 5, 10, 15, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 500, 1000 and 2000  $\mu\text{m}$ . The values of  $\alpha$  were obtained according to the sand contents of the samples, the details of which are included in Table 2. The values of  $\beta$  were obtained by substituting the  $S_{SA}$  values predicted using Eq. (120) into Eq. (119). Then, the PoSD was predicted using Eqs. (86)-(108). Finally, the SWC was estimated using the methods described in Sect. 3.3.

25 The SWC was also predicted using the traditional method presented in Sect. 2. In the traditional method, the predicted PoSD was equivalent to the PSD in Eq. (1) and was substituted into Eq. (3) to obtain the water content. The corresponding suction heads were predicted using Eqs. (2) and (54).

A scaling approach proposed by Meskini-Vishkaee et al. (2014) was used to compare with the proposed method to demonstrate the prediction performance. The detailed calculation procedures were described by Meskini-Vishkaee et al. (2014).

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The van Genuchten equation (Eq. (142)) was used to fit the SWC data calculated via the traditional method and the improved model (Genuchten, 1980):

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[ \frac{1}{1 + (a\psi)^n} \right]^m$$

(142)

where  $\theta$  is the water content ( $\text{cm}^3 \text{cm}^{-3}$ ),  $\theta_r$  is the residual water content ( $\text{cm}^3 \text{cm}^{-3}$ ), and  $a$ ,  $n$ ,  $m$ , and  $\theta_r$  are fitting parameters.

The 292 samples exhibited good fits with an average  $r^2$  value of greater than 0.999.

For each set of predictions, the agreement between the predicted water content  $\theta_p$  and the measured water moisture content  $\theta_m$  was expressed in terms of the root mean square error ( $E_{RMS}$ ), which is given by

$$E_{RMS} = \sqrt{\frac{1}{N} \sum_{i=1}^N (\theta_p - \theta_m)^2}$$

(153)

where  $N$  is the number of measured data points.

## 4.2 Results

The predicted and measured SWCs in Fig. 56 showed that the improved method exhibited good fits with the measured data in the entire range of the SWC; moreover, the proposed method was clearly better than the traditional method and the scaling approach, especially at the dry range (the other 2548 samples are listed in Fig.S3 in the supporting information). The scaling approach, which improved the performance of original MV-VG model via scaling the  $n$  parameter in van Genuchten equation, performed better than the traditional method here for clay (code:1360), loamy (code: 3190) and loamy sand (code: 3160). However, it performed worse for coarse-textured soil (eg. sand-code: 3144), which may result from the relative small scaling degree of the parameter  $n$  and the poor fitting of the fitting equation to measured PSD data in their study. In general, the improved method here applied well to a wide range of soils, while the scaling approach performed better for fine- and medium-textured soils.

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Table 4 showed the  $E_{RMS}$  of the improved method, the scaling approach and the traditional method for samples used in model validation. The  $E_{RMS}$  values range from 0.017 to 0.054 for the improved method (with an average of 0.0287), and from 0.026 to 0.060 for the scaling approach (with an average of 0.037) and from 0.040 to 0.106 for the traditional method (with an average of 0.06157). Among the three methods mentioned above, the improved method provided the best predictions and the traditional method performed worst.

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The accuracy of an SWC predicted using the improved method depends on the accuracy of the corresponding predicted pore volume fractions. The calculated and measured pore volume fraction curves in Fig. 6 indicate that the predicted pore volume fraction curves using the improved method are more similar to the measured data than those predicted using the traditional method, thereby showing that the proposed method performed better. The errors in the predicted pore fraction using the traditional method mainly occur at the minimum pore size ( $d \leq 0.6 \mu\text{m}$ ), while the proposed method greatly improves the volume fraction at ~~this the minimum~~ pore size and consequently improves the water content in the high suction range. These improvements are mainly attributed to the pore model containing slit-shaped spaces, demonstrating that this pore model is better for predicting the SWC from the PSD than the concept of a bundle of cylindrical tubes.

### 4.3 Discussions

#### 4.3.1 The suction head calculation in slit-shaped spaces

~~When capillary water coexist with adsorptive water in the narrow pores, the capillary force and surface force including ionic-electrostatic, molecular, structural, adsorption ones contribute to the potential energy of water in slit-shaped pore~~ (Tuller et al., 1999; Iwamatsu and Horii, 1996). ~~When considering the capillary forces only, the drainage potential in slit-shaped pore is given as Eq.(7) (Derjaguin and Churaev, 1992), while the applicability of this formula is limited by the width of the slit. A correction of taking into account the effect of adsorption force at the slit surfaces will have to be made for thin slit-shaped spaces. (Tuller and Or, (2001) defined a critical slit spacing ( $ad^*$ ) by Eq.(16) that would classify slit sizes responding to capillary drainage and adsorption dominated drainage. In case of slit spaces greater than  $ad^*$ , the capillary-based slit drainage would be applied.~~

$$\alpha d^* = \sqrt{-\frac{9A_{svl}}{4\pi\sigma}} \quad (16)$$

where,  $A_{svl}$  is the Hamaker constant for solid-vapor interaction through the intervening liquid, usually set as  $-6.0\text{E}-20 \text{ J}$  (Tuller and Or, 2001). The value of  $ad^*$  is 0.591 nm, it means that for slit-shaped spaces greater than 0.591 nm, the Eq.(7) could be applied to calculate the drainage potential.

Besides, in our study, the calculated suction head was small than 5000cm  $\text{H}_2\text{O}$ , under which all slit-shaped spaces were filled with water, therefore the capillary pressure could be considered as the dominant acting forces, and Eq.(7) could be applied.

#### 4.3.2 The effects of estimated $S_{SA}$ values

The  $S_{SA}$  values estimated using Eq. (12) could affect the accuracy of the predicted SWC. Fig. 7 shows that an overestimation of the  $S_{SA}$  would prompt the dry range of the SWC curve to move in the direction of a larger water content, and vice versa. ~~When the estimated error in the  $S_{SA}$  was  $\pm 20\%$  of its accurate value, a relatively small error appeared between the calculated and measured SWCs.~~ When the estimated  $S_{SA}$  value was altered by 10% and -10% of its accurate value for the

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loamy sand (code: 3170), the water contents with respect to the highest suction head were higher and lower, respectively, by approximately  $0.007 \text{ cm}^3 \text{ cm}^{-3}$  than those of the original SWC. For the clay (code: 4680), the water contents were higher and lower by approximately  $0.009 \text{ cm}^3 \text{ cm}^{-3}$  at the same 10% and -10% alterations, respectively. Consequently, for the coarse-textured soil, the water content and prediction error of the SWC changed relatively little for the same degree of change of the  $S_{SA}$ . This effect may contribute to the lower  $S_{SA}$ -value for this texture than the fine-textured soil. Fig. 7 also showed that a relatively small error appeared between the calculated and measured SWCs when the estimated  $S_{SA}$  error was within 20 %.

Previous work showed that the  $S_{SA}$  of soil is closely dependent upon the soil texture and that it could be estimated from the soil media data and PSD (Sepaskhah and Tafteh, 2013; Resurreccion et al., 2015). The method used to estimate the  $S_{SA}$  in Sect. 3.2 was presented by (Sepaskhah et al., 2010), who estimated the  $S_{SA}$  based on the geometric mean particle size diameter as shown in Eq. (129) with an  $r^2$  value of 0.88. Moreover, the appropriateness of this equation was validated using 64 soil samples by (Fooladmand, 2011). Sepaskhah et al. (2010) pointed out that the deviations increased distinctly for measured  $S_{SA}$  greater than  $200 \text{ m}^2 \text{ g}^{-1}$ . In proposed method, the estimated  $S_{SA}$  is mainly used to gain the parameter  $\alpha$  and  $\beta$  and to estimate the volume fraction of the slit-shaped spaces, thus the estimation accurate of  $S_{SA}$  influence the dry range of the SWC curve (Fig. 7), equivalently the degree of improvement of predicted SWC. Overall there are always different levels of improvement comparing with the SWC predicted by the traditional method. Therefore, this equation is capable of estimating the  $S_{SA}$ , but Continually putting more effort should be directed toward developing a more accurate transformation from soil physical properties to  $S_{SA}$  to further improve the prediction of the SWC.

#### 4.3.32 Physical meanings of the parameters

Since the central pore diameter  $d$  is proportional to the corresponding particle diameter  $D$ , the slit width  $ad$ , slit length  $\beta d$  and specific surface area  $S_{SAi}$  of each unit cell are associated with the particle size. The calculated values of  $ad$ ,  $\beta d$  and  $S_{SAi}$  of clay, silt, fine sand and coarse sand particles for the loamy sand (code: 3170) are listed in Fig. 8. The results confirm that pores formed by bigger soil particles are large with a correspondingly large slit width  $ad$ ; this is similar to the results in (Or and Tuller, 1999), and the values are of the same order of magnitude. It is common knowledge that larger soil particles tend to have large surface areas, and therefore, the slit length formed by the contact of soil particle edges should be relatively long, leading to the positive relationship between the slit length  $\beta d$  and the particle diameter as shown in Fig. 8. This result is different from that in (Or and Tuller, 1999), where the slit length  $\beta d$  was inversely proportional to the particle diameter. In addition, the  $S_{SAi}$  of the  $i$ th particle fractions decreased with an increase in the particle diameter, which is consistent with the findings of (Or and Tuller, 1999) and is in accordance with the general understanding of the  $S_{SA}$ .

## 5 Conclusions

The traditional models employed to translate the PSD into the SWC underestimate the water content in the dry range of the SWC. The errors originate from a setting that the cumulative PoSD equal to the corresponding PSD which resulted in an

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underestimate of the pore volume fraction of the minimum pore diameter range and consequently the water content in the dry range of the SWC. If slit-shaped pore spaces are taken into consideration when estimating PoSD with a pore model comprising a circle-shaped central pore connected to slit-shaped spaces, ~~the pore volume fraction of the minimum pore diameter range will be accordingly increased if slit-shaped pore spaces are taken into consideration when estimating PoSD with a pore model comprising a circle-shaped central pore connected to slit-shaped spaces;~~ therefore, the SWC can be more accurately predicted from the PSD. The estimation of the  $\alpha$  and  $\beta$  values is a key step to predict the SWC in the proposed method. The  $\alpha$  values were obtained using 48 measured soil samples, and those values served as input parameters while predicting the SWC; then, the  $\beta$  values were readily calculated using a constraint on the estimated  $S_{SA}$ . The validation results illustrate that the SWCs predicted using the proposed method provided the best predictions of the SWCs, closely followed by the scaling approach, and the traditional method performed worst.  ~~demonstrated a good fit with the measured data and the proposed method performed better than the traditional method, especially in the dry range of the SWC.~~

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*Competing interests.* The authors declare that they have no conflicts of interest.

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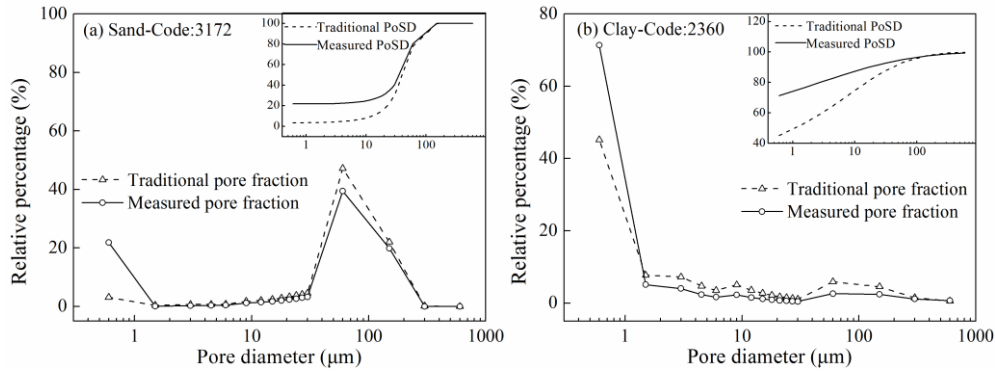
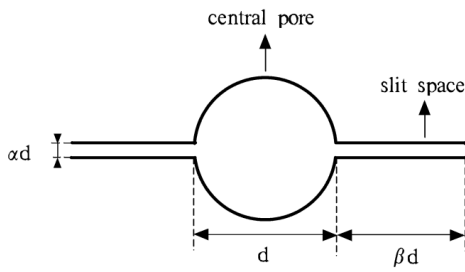


Figure 1: Measured vs. calculated pore volume fraction curves for (a) sand (code: 3172 ) and (b) clay (code: 2360). The measured and calculated PoSDs are embedded in the tops of the figures.



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Figure 2: Pore space geometry model containing two slit-shaped spaces ( $d$  denotes the diameter of the central pore, and  $\alpha d$  and  $\beta d$  denote the widths and lengths of the slit-shaped spaces, respectively).

	Formed pores	PSD	Volume fraction of slit-shaped spaces	Volume fraction of pores
$d_1 \leq 0.6 \mu\text{m}$		$\omega_1$		$v_1 = \omega_1 + \zeta_2 + \dots + \zeta_i$
$d_2$		$\omega_2$	$\zeta_2$	$v_2 = \omega_2 - \zeta_2$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$d_i$		$\omega_i$	$\zeta_i$	$v_i = \omega_i - \zeta_i$

Figure 3: Schematic of the procedure used to calculate the pore volume fraction.

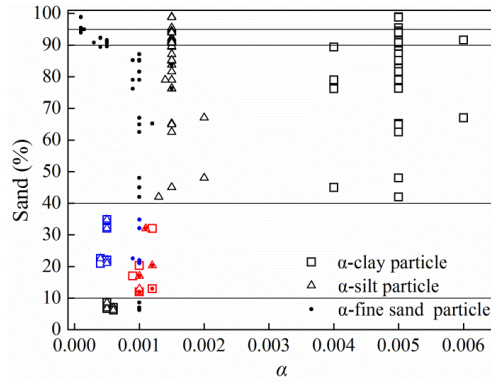


Figure 4: The  $\alpha$  values for the 48 soil samples with different sand contents. The  $\alpha$  values for specific samples of clay, silt, and fine sand are listed in Figure 4 except those of coarse sand particles, which are the same value of 0.0004 for all of the samples. For the samples with sand contents ranging from 10-40%, two sets of  $\alpha$  values are observed. The  $\alpha$  values for silt contents of less than and more than 50% are highlighted in red and blue, respectively, thereby reflecting the dominant functions of silt or clay particles on the hydraulic properties of the typical samples.

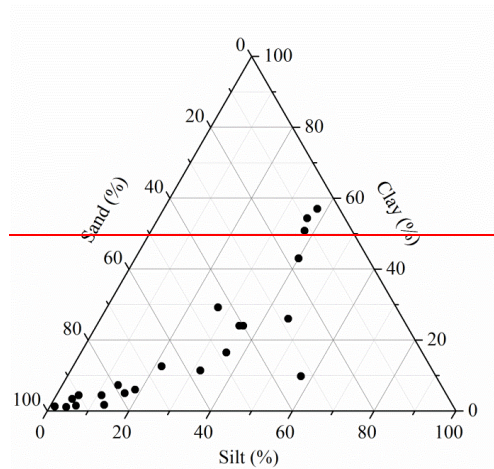
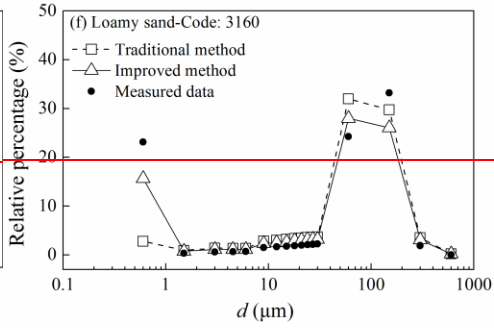
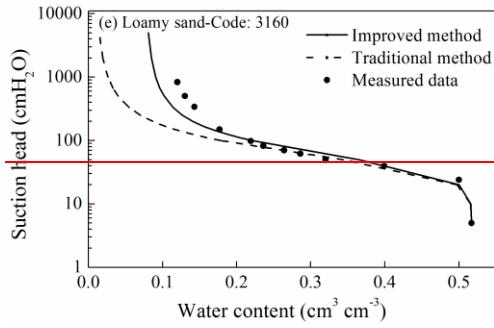
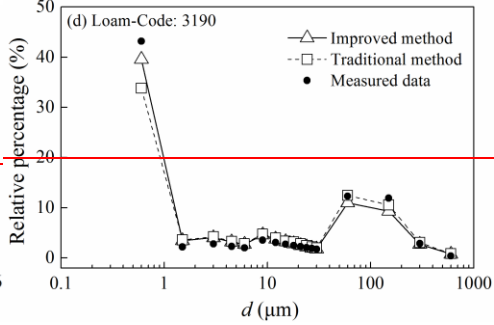
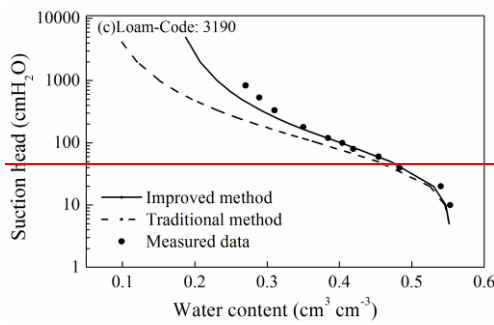
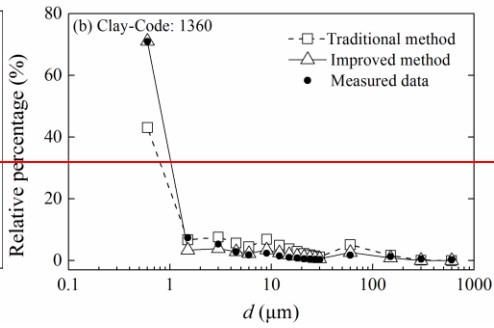
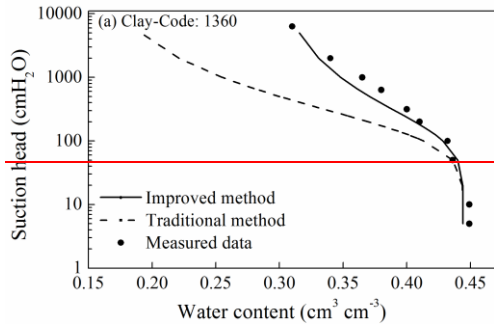


Figure 5: Textural distribution of the 22 soil samples for the model validation.



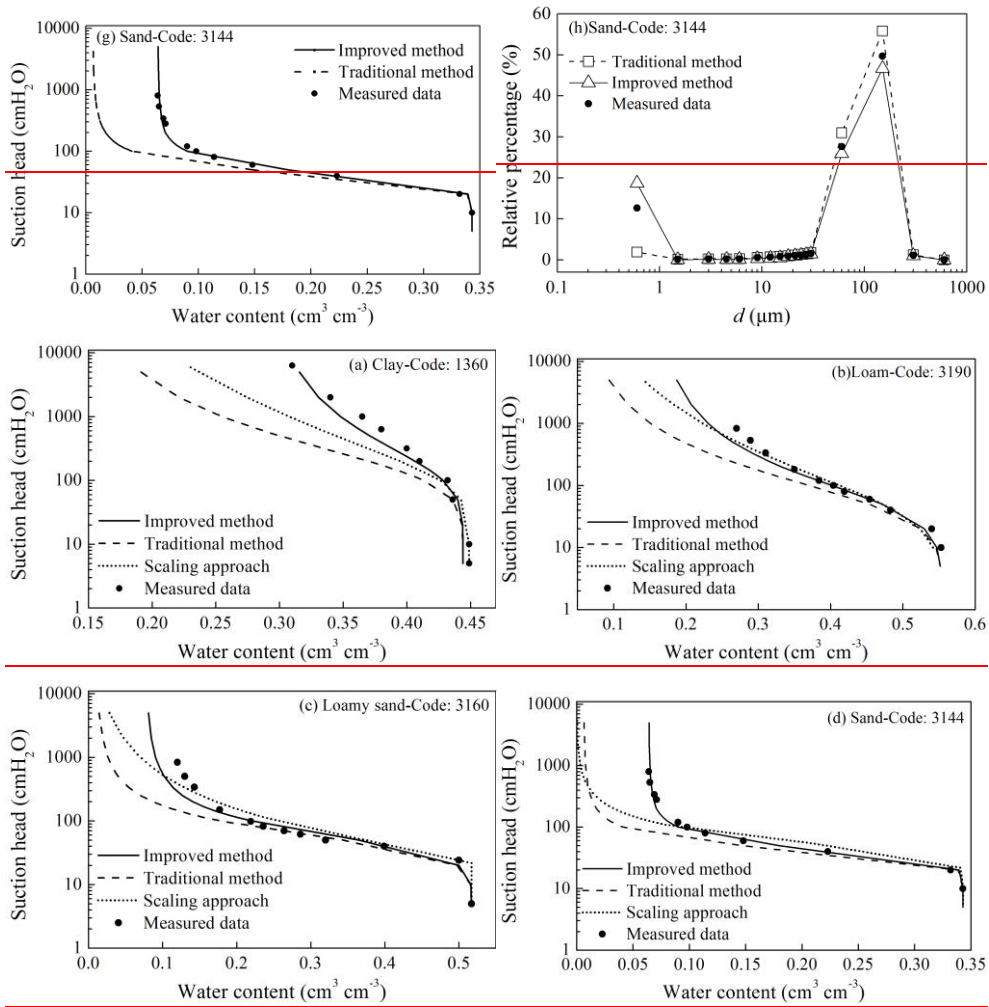
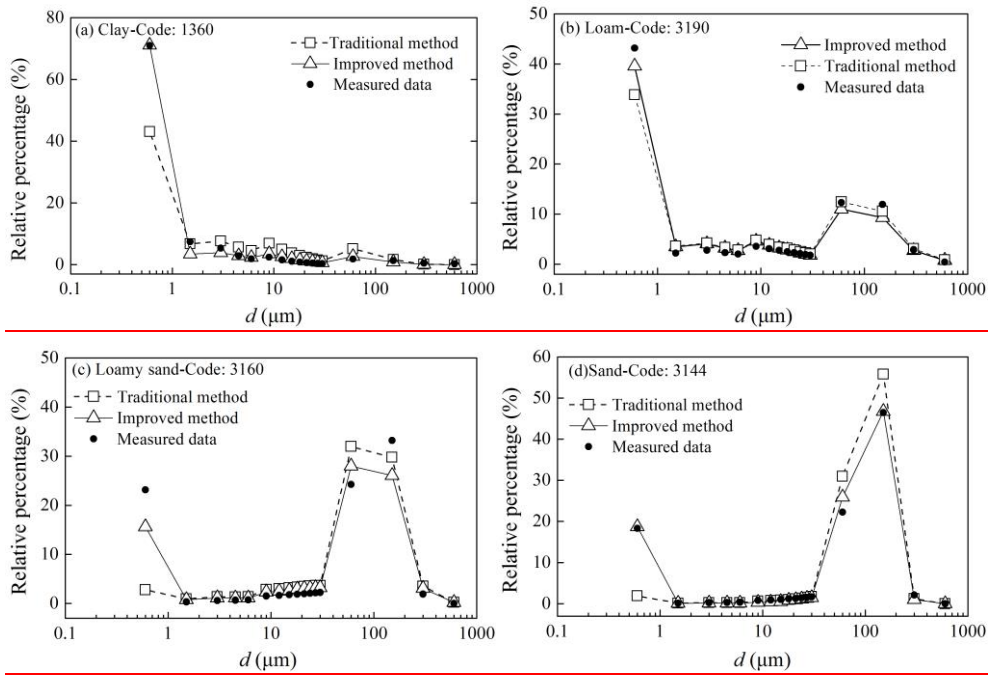


Figure 56: Measured and predicted SWC curves (left) in addition to measured and predicted pore volume fraction curves (right) for clay (code: 1360), loam (code: 3190), loamy sand (code: 3160) and sand (code: 3144).



**Figure 6: The measured and predicted pore volume fraction curves using improved method and traditional method for clay (code: 1360), loam (code: 3190), loamy sand (code: 3160) and sand (code: 3144).**

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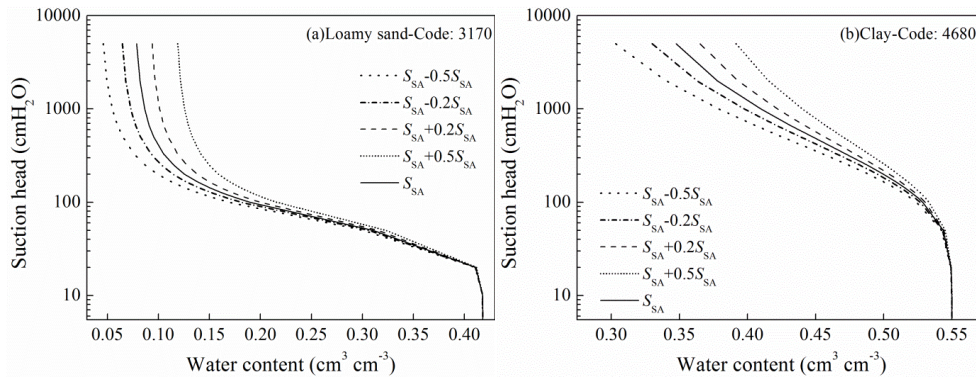




Figure 7: The effects of an alteration of the estimated  $S_{SA}$  on the SWC for (a) loamy sand (code: 3170) and (b) clay (code: 4680).

$S_{SA}$  denotes the accurate value of the specific surface area.


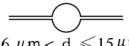
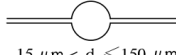
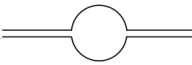
Loamy sand–Code: 3170		$S_{SA}=8.19\text{m}^2\text{g}^{-1}$		
Particle size fraction	Formed pores	$\alpha d$ (m)	$\beta d$ (m)	$S_{SAi}$ ( $\text{m}^2\text{g}^{-1}$ )
Clay	 $d \leq 0.6 \mu\text{m}$	3E-9	0.00004	4.98
Silt	 $0.6 \mu\text{m} < d \leq 15 \mu\text{m}$	1.4E-8	0.00056	1.91
Fine sand	 $15 \mu\text{m} < d \leq 150 \mu\text{m}$	8.4E-8	0.0051	1.29
Coarse sand	 $150 \mu\text{m} < d \leq 600 \mu\text{m}$	1.2E-7	0.0178	0.006

Figure 8: The calculated slit width  $\alpha d$ , slit length  $\beta d$  and  $S_{SAi}$  for loamy sand (code: 3170).

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Table 1: Codes and textural classes of the 48 soils selected from UNSODA

UNSODA codes	Textual class
4681, 4680, 2362, 2360, 1400, 1383, 4121, 1361, 2340	Clay
3191, 1091, 2530, 2531	Loam
2102, 3150, 3161, 3171, 1160, 3170, 3130, 1031, 4011, 4020	Loamy sand
1464, 1466, 2100, 3340, 4650, 3142, 1050, 1023, 3141, 3163, 3164, 3165, 3172, 4051, 4520, 4521	Sand
3202	Sandy clay loam
3200, 3203, 4162	Sandy loam
4042, 4180, 4070, 4673, 1341	Silt loam

10

Table 2: The estimated values of  $\alpha$  for various soil textures

Sand content (%)	Silt content (%)	$\alpha$			
		Clay $D \leq 2 \mu\text{m}$	Silt $2 \mu\text{m} < D \leq 50 \mu\text{m}$	Fine sand $50 \mu\text{m} < D \leq 500 \mu\text{m}$	Coarse sand $500 \mu\text{m} < D \leq 2000 \mu\text{m}$
0-10		0.0005	0.0005	0.001	0.0004
10-40	0-50	0.001	0.001	0.001	0.0004
	50-100	0.0005	0.0005	0.001	0.0004
40-90		0.005	0.0015	0.001	0.0004

90-95	0.005	0.0015	0.0005	0.0004
95-100	0.005	0.0015	0.0001	0.0004

**Table 3: Codes of the 292 soil samples selected from UNSODA for the model validation**

UNSODA codes	Textual class
1360, 4120, 2361, 3282, <u>1320</u>	Clay
3190, 1370	Loam
3160, 3152, 1030, 1090, 4010	Loamy sand
3155, 3144, 1463, 3132, 4000	Sand
4620, 4621, <u>1102, 2341</u>	Sandy clay loam
3290, 3310	Sandy loam
4531, 4510	Silt loam
<u>3031, 3032, 1372, 1362</u>	<u>Clay loam</u>

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**Table 4: The root mean square errors ( $E_{RMS}$ ) of the SWC predicted using ~~both~~ the improved method, the scaling approach and the traditional method**

Soil texture	Number of soil sample	$E_{RMS}$		
		Improved method	<u>Scaling approach</u>	<u>Traditional method</u>
Clay	<u>54</u>	<u>0.022</u>	<u>0.032</u>	<u>0.056</u>
<u>Clay loam</u>	<u>4</u>	<u>0.034</u>	<u>0.041</u>	<u>0.079</u>
<u>Sandy clay loam</u>	<u>4</u>	<u>0.032</u>	<u>0.046</u>	<u>0.072</u>
Loam	2	0.054	<u>0.060</u>	<u>0.106</u>
Loamy sand	5	0.020	<u>0.026</u>	<u>0.048</u>
Sand	5	0.017	<u>0.028</u>	<u>0.042</u>
Sandy loam	<u>2</u>	0.046	<u>0.049</u>	<u>0.068</u>
Silt loam	<u>2</u>	0.024	<u>0.031</u>	<u>0.040</u>

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