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Wading through a swamp of complete confusion: how to choose a method for estimating soil water retention parameters for crop models ☆

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Abstract

A minimum input for water dynamics simulation in crop models are soil water content at field capacity drained upper limit (DUL), wilting point, lower limit (LL) and, often, saturation (SAT). Eight methods for estimating these water retention parameters were compared using the following procedure: (1) Stepping through the texture triangle in increments of 1% clay and 1% sand, LL, DUL and SAT were calculated for all possible texture combinations (from 0 to 100% sand, giving > 5000 cases, though not all could be used for all methods); results were grouped by soil type in the USDA classification system. (2) The estimated LL and DUL were compared with field-measured data from across the USA. (3) (Imaginary) soils with a homogenous profile of each of these texture combinations were defined and the DSSAT crop model was run with 11 years of weather data to estimate soybean yield. The discrepancy between estimation methods for water retention parameters was so big that it is hard to make recommendations on which method to use for which soil. Yet, an analysis with a set of field-measured data showed that the Saxton method performed best for LS, SL, L and SIL soils, with a RMSE < 0.018. Using these data as input to the CROPGRO-Soybean model (which is part of DSSAT) showed a worrisome variability among methods in simulated crop yield. The dataset of both field-measured and lab-measured values of LL and DUL showed very different estimates, shedding doubt on the value of lab-measured water retention data for parameterizing a crop model. Several methods showed inaccuracies in their equation structure.

Keywords: Field capacity; Pedotransfer functions; Wilting point; Estimation method; Crop models

1. Introduction

With the increased use of crop models in agricultural research and as decision-support tools for farm managers, there is an increased demand for procedures that can assist in the parameterization of such models. Models dealing with crop production generally need input data on soil and weather conditions, crop characteristics, the oc-

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Nomenclature

DUL	drained upper limit, or field capacity
DUL10, DUL33	DUL calculated at, respectively, −10 and −33 kPa
DULfield	DUL calculated from field measurements
DULvar	DUL calculated at a variable (texture-dependent) matric potential
LL	lower limit, or wilting point
SAT	saturation point
AWHC	available-water-holding capacity, or plant-extractable water content (= DUL − LL)
AWHC10, AWHC33, AWHCfield, AWHCvar	AWHC as calculated with, respectively, DUL10, DUL33, DULfield and DULvar
POR	soil porosity
pF curve	soil water retention curve
PTF	pedotransfer function
SOM	soil organic matter
C_{org}	soil organic carbon content
APD	adjusted particle density
BD	bulk density
K_{sat}	hydraulic conductivity
θ	volumetric water content
θ_s	volumetric water content at saturation
ψ	matric potential
Soil classification	
C	clay
CL	clay loam
LS	loamy sand
S	sand
SC	sandy clay
SCL	sandy clay loam
SI	silt
SIC	silty clay
SICL	silty clay loam
SIL	silt loam
SL	sandy loam

currence of pests and diseases, and management. Such models can either be used at a fine scale, e.g., as a research tool and for precision agriculture, or at a coarser scale, such as for regional/continental food-security forecast (Van Keulen and De Milliano, 1984; Thornton et al., 1995), or predicting potential effects of climate change on crop production in (part of) a country (Jagtap and Jones, 2002). For a small area, soil parameters may be obtained by sampling, but measuring soil conditions such as texture, organic-matter content, available-water-holding capacity (AWHC) and saturated conductivity for a complete continent at a fine spatial resolution, is practically impossible.

Alternative approaches are therefore needed, in which soil characteristics that are not readily available are expressed in terms of basic soil data that are more widely available through soil surveys. Bouma (1989) introduced the term pedotransfer function (PTF) for this purpose. Such functions are now used in agronomy, soil-quality assessment and contaminant hydrology (Pachepsky et al., 1999). Many PTFs for estimating soil hydraulic properties have been published over the years (see overviews in Rawls et al., 1991; Timlin et al., 1996); the latter authors reported 49 methods and estimated that this covers only about 30% of the total.

The application of such indirect methods for predicting the hydraulic properties of a soil may have a sufficient level of precision for some practical applications (Wösten, 1997), but for crop model applications a higher level of precision is needed, as these are some of the parameters the crop model is most sensitive to. An incorrect estimate may make the difference between a purely academic simulation or one that tries to mimic reality. Crop models generally need input data by soil layer on soil-water retention, such as the volumetric water content ($cm^3[H_2O]\ cm^{-3}[soil]$) at permanent wilting point lower limit (LL), at field capacity drained upper limit (DUL) and at saturation (SAT). The saturated conductivity K_{sat} ($cm\ h^{-1}$) is often also needed.

According to Rawls et al. (1991), soil physical properties used to derive water retention can be grouped into four categories: (1) soil particle size, (2) hydraulic characteristics, (3) morphological properties, (4) chemical properties. Often, particularly for large-scale crop model applications, the soil texture is all that is available, sometimes combined with bulk density (BD) and/or soil-organic-matter (SOM) content. Approaches followed to develop a PTF vary from multiple regression techniques (e.g. Gupta and Larson, 1979), estimating parameters for equations that express the soil-water content θ as a function of the soil-water potential ψ (e.g. Saxton et al., 1986), or physico-empirical models in which the pF curve is derived from physical attributes such as particle size (e.g. Arya and Paris, 1981). Pachepsky et al. (1999) describe recent developments in the estimation of soil-water retention curves, involving artificial neural networks (e.g. Minasny et al., 1999), extended nonlinear regression (e.g. Scheinost et al., 1997), and group method of data handling (GMDH; e.g. Pachepsky et al., 1999). Some of these methods allow inclusion of one or more measured data points—generally θ at -33 and/or -1500 kPa (e.g. Rawls et al., 1982)—which may improve the estimate (Williams et al., 1992). Further improvements may be obtained by deriving PTFs for specific textural classes and then combining them into one set of equations (Pachepsky et al., 1999).

A number of authors have developed PTFs based on only data from a specific region and intended for regional application (e.g. Hall et al., 1977, for England and Wales; De Jong, 1982, for Canada; Wösten and Van Genuchten, 1988, for the Netherlands; Bastet et al., 1997, for France; Vereecken et al., 1989, for Belgium; Minasny et al., 1999, for Australia). Often though these methods are used in a wider setting, such as the Ritchie et al. (1987) method, which is used worldwide, but is based on data in the USA only. The performance of a PTF may vary with pedological origin of the soil on which it was developed (Bastet et al., 1997; Minasny et al., 1999), and the PTF may not be directly transferred to elsewhere. Such a wide application of regional PTFs may thus be a source of errors in simulation model results.

Some PTFs only provide equations for selected values of the matric potential (e.g. Rawls et al., 1982, for 12 matric potentials) sometimes only LL, DUL and SAT (e.g. Ritchie et al., 1987); others estimate a few points, which are then used as input in functions for estimating the complete water retention curve (e.g. Rawls and Brakensiek, 1985; Baumer and Rice, 1988), using functions like those of Brooks and Corey (1964), or Van Genuchten (1980).

Kern (1995) compared 6 of these methods with data from nearly 6000 pedons from across the USA; Williams et al. (1992) did a similar exercise with 4 estimation methods for a site in Oklahoma. Timlin et al. (1996) compared 2 estimation methods for four locations in Colorado (USA) and also evaluated how the estimation methods compared with measured data, if used as input to the GLYCIM crop model. All the estimation methods these authors compared were based on measurements in a laboratory with a pressure-plate apparatus or another technique; the data they were compared with were also lab-measured. It is well known (Van Bavel et al., 1968b; Ritchie, 1981; Ratliff et al., 1983) that what scientists define as 'field capacity' or 'wilting point' in a laboratory may be very different from what a plant experiences in the field. The only estimation methods we know of that are based on field-measured data on LL and DUL, are those of Ritchie et al. (1987, 1999). These methods, though from the same lead author, are quite different, but used the same dataset with 401 observations from 15 US states (Ratliff et al., 1983; Ritchie et al., 1987).

The objective of our work was to compare several commonly used methods for estimating the critical model parameters LL, DUL and SAT for soils in the USA, and evaluate their accuracy for different soil types or under certain conditions of data availability. We used field-measured soil-water retention data to compare the results from the different methods with, as we believe that this is closer to reality. This work was part of a project on the impact of methodology on the accuracy of climate-change predictions on agriculture in the USA; therefore, only estimation methods developed with US soils were used.

2. Materials and methods

2.1. Methods compared

Eight PTFs for calculating soil-water-retention characteristics were compared:

1) Rawls et al. (1982)
2) Rawls and Brakensiek (1985) combined with Brooks and Corey (1964)
3) Rawls and Brakensiek (1985) combined with Campbell (1974)
4) Rawls and Brakensiek (1985) combined with Van Genuchten (1980)
5) Saxton et al. (1986)
6) Baumer and Rice (1988)
7) Ritchie et al. (1987)
8) Ritchie et al. (1999)

Table 1 shows the necessary input data for each of these.

Rawls et al. (1982) used a step-wise regression technique to derive a set of equations for the relationship between matric potential ψ and volumetric water content θ for three levels of data availability: (1) texture, SOM content and BD; (2) texture, SOM, BD and (laboratory-) measured θ at -1500 kPa; (3) texture, SOM, BD and measured θ at -33 and -1500 kPa. Different regression coefficients were derived for 12 matric-potential values, under the above-mentioned input conditions (some matric potentials do not have regression coefficients for all input levels). Only option (1) was used here. This method also has been published by Rawls and Brakensiek (1989). The authors did not define limitations on the applicability of this method, but for our analysis the same limits as in Saxton et al. (1986) were applied, as both authors used the same dataset for their analyses. This method is cited in the text as the Method_Rawls.

Saxton et al. (1986) used the data of Rawls et al. (1982) to derive equations that cover the whole range of matric-potential values, instead of only 12 selected values. They used the regression approach of Rawls that is least input-data demanding, from which they removed the influence of the BD and in which the SOM content was fixed at 0.66%, the average value reported by Rawls et al. (1982). The Saxton approach thus only needs texture (sand, clay) data. This method may be applied for soils of $5\% \leqslant \text{sand} \leqslant 30\%$ with $8\% \leqslant \text{clay} \leqslant 58\%$, and $30\% \leqslant \text{sand} \leqslant 95\%$ with $5\% \leqslant \text{clay} \leqslant 60\%$. It is cited in the text as the Method_Saxton.

Rawls and Brakensiek (1985) developed regression equations to estimate various parameters that can be used with several estimation techniques for soil-water retention and hydraulic-conductivity, such as Brooks and Corey (1964), Campbell (1974) and Van Genuchten (1980). The parameter estimates—e.g., bubbling pressure, residual water content and effective SAT—are based on the percentages of sand and clay and the porosity of the soil. We used this method with all three above-mentioned water retention estimation techniques. This method also has been published by Rawls and Brakensiek (1989) and Rawls et al. (1991). This method may be applied for soils with $5\% \leqslant \text{clay} \leqslant 60\%$ with $5\% \leqslant \text{sand} \leqslant 70\%$. It is cited in the text

Table 1
Input data needed for the various methods for estimating soil water retention parameters

	Method cited as	Sand silt clay	Sand sub fraction	Bulk density	SOM	Clay activity	Compaction
Rawls et al. (1982)	Method_Rawls	*		*	*		
Rawls and Brakensiek (1985)+Brooks and Corey (1964)	Method_Rawls–Brakensick+Brooks–Corey	*		* ([a])	* ([b])		
Rawls and Brakensiek (1985)+Campbell (1974)	Method_Rawls–Brakensiek+Campbell	*		* ([a])	* ([b])		
Rawls and Brakensiek (1985)+Van Genuchten (1980)	Method_Rawls–Brakensiek+VanGenuchten	*		* ([a])	* ([b])		
Saxton et al. (1986)	Method_Saxton	*					
Baumer and Rice (1988)	Method_Baumer–Rice	*	*	*	*	*	*([c])
Ritchie et al. (1987)	Method_Ritchie1987	*		*	*		
Ritchie et al. (1999)	Method_Ritchie1989	*		* ([d])	*		

[a] BD used for calculating the porosity, not in the regression equations for calculating θ.
[b] SOM used for calculating porosity, not in the regression equations for calculating θ.
[c] Compaction is by default set to 'no compaction'.
[d] BD used for converting gravimetric to volumetric water content, not in the regression equations for calculating θ.

as the Method_Rawls–Brakensiek, with a follow-up method of Brooks–Corey, Campbell or Van Genuchten.

Baumer and Rice (1988) introduced a method that calculates θ for 4 specific matric potentials (0, −33, −1500 kPa and residual water content), which are then used for fitting a pF curve with the RETC program (Van Genuchten et al., 1991). This method differs from the others in that it not only uses clay, sand and SOM, but also (1) several more-detailed texture classes: very fine, fine, medium, coarse and very coarse sand; (2) clay activity (the ratio of cation exchange capacity of the soil minerals to the percentage clay; Baumer and Brasher, 1982); (3) soil compaction.

We used a clay activity of 0.3, which is mainly found in the far eastern zone of the USA according to the map the authors show (the rest of the country has higher values) and a default of 'no compaction'. This approach was originally part of the DRAINMOD program (Baumer et al., 1987; Baumer and Rice, 1988; Baumer, 1990) and is now built into the MUUF program (Map Unit Use Files; Baumer et al., 1994), the code of which can be downloaded (ftp://ftp.wcc.nrcs.usda.gov/water_mgt/muuf/). The authors did not define limitations on the applicability of this method.

Though the DUL with this method is initially calculated at the commonly used −33 kPa, it is recalculated at a matric potential that varies by soil type, after having computed the full pF curve. For sandy soils, sandy loams and loamy sands it uses the subclasses of the sand (very coarse, coarse, etc.); the newly calculated DUL matric potential can either be higher or lower than −33 kPa (−10.2 to −46 kPa). For such a soil-dependent matric potential, the soil first has to be classified according to the US soil classification system. A utility in the MUUF program addresses this, though it was slightly modified to cover the full range of texture combinations.

Not all soils under study had the sand sub fractions available; these were then set to default values of 80% medium sand, 10% coarse sand 10% fine sand (the other subclasses were set to zero). This resulted in sandy, sandy loam and loamy sand soil being classified in the average class (i.e. a 'sandy loam' was not reclassified as either 'very-fine/fine/coarse/very coarse sandy loam', but as the modal 'sandy loam'). This method is cited in the text as the Method_Baumer–Rice.

Ritchie et al. (1987) developed a method for calculating wilting point, field capacity and SAT, which needs input on texture, SOM and BD. This method was specifically meant for crop models that require only LL, DUL and SAT soil-water retention data. Their method may be applied to any soil type, besides organic soils or tropical soils with large amounts of low-activity clays. This method has also been presented in slightly different form, by Ritchie et al. (1986, 1990) and Ritchie and Crum (1989). An important difference with all other methods discussed here (except Ritchie et al., 1999) is that Ritchie et al. (1987) was derived from field-measured instead of lab-measured water retention data, based on a large survey with sampling points across the USA (Ratliff et al., 1983; Ritchie et al., 1987). The authors did not define limitations on the applicability of this method. This method is cited in the text as the Method_Ritchie1987.

Ritchie et al. (1999) used the same dataset on field-measured water retention data, but generalized assumptions for estimating LL, DUL and SAT. DUL was made a function of the soil's sand/clay ratio, BD and SOM, while the plant-extractable water content depends only on the soil's sand content; the LL is then calculated by subtracting these two (i.e. θ at wilting point = θ at field capacity minus plant-extractable water content). Plant-extractable water content is set to almost the same value across most soils (≈ 0.132 cm^3 cm^{-3}, only depending on the SOM content), except those with a high sand content. A computer utility was released by the authors (SWLIMITS), in which the user provides texture, SOM and BD, and gets the estimated LL, DUL and plant-extractable water; this program can be downloaded from http://nowlin.css.msu.edu/. The authors did not define limitations on the applicability of this method, but it cannot be used for 0% clay or 0% sand, given the mathematical relationships in the equations (e.g. division by clay). This method is cited in the text as the Method_Ritchie1999.

2.2. How the comparison was done

2.2.1. Step 1

The volumetric water content at LL, DUL and SAT was calculated for the whole range of textures from 0% sand to 100% sand, with texture increments of 1% (thus 0% sand/0% clay/100% silt, 1% sand/0% clay/99% silt, 1% sand/1% clay/98% silt, 1% sand/98% clay/1% silt..., 100% sand/0% clay/0% silt, 0% sand/100% clay/0% silt).

The SOM content of the soils was set to 0.66%, reported by Rawls et al. (1982) as the average for the USA and also used by Saxton et al. (1986). As soils of different texture generally have a different BD, a common value could not be used. Thus, BD was estimated for each soil according to Rawls and Brakensiek (1985, 1989): first the mineral BD (i.e. minerals plus pores, but without SOM) was taken from Fig. 1 of the 1985 article, which was then corrected for the SOM content by weighting the contributions of minerals and SOM. The adjusted particle density APD (i.e. minerals plus SOM, but without pores) was calculated, after which porosity was calculated as 1-BD/APD (Baumer and Rice, 1988). Not all methods give an estimate for SAT or some give an estimate that results in impossible values (See Section 3, A critical note). For those methods, SAT was set to 95% of the porosity. In all calculations soil texture was defined according to the USDA system, where clay <0.002 mm, silt $=0.002$–0.05 mm, and sand $=0.05$–2.0 mm.

2.2.2. Step 2

The calculated LL, DUL and SAT from step 1 were compared with field-measured data, extracted from Ratliff et al. (1983) and Ritchie et al. (1987). At greater depths, the LL tended to increase and approach the water content of soil layers that were not affected much by root water uptake. Only those layers were included that were likely to be within the reach of the roots, which depth very conservatively was taken as 100–120 cm. Layers that showed an LL increase with depth were excluded (cf. Van Bavel et al., 1968a). The authors themselves had already excluded the topsoil layer ($\approx$10–15 cm) from consideration, as this layer often dries out much more than the rest of the soil. This left 272 pedons from the original set of 401.

Another dataset used was the one of Braga (2000), in which a maize field in Michigan, USA, was split into 43 small plots. In each plot the water profile was measured weekly during 1997 and 1998 by neutron probe, in steps of 15 cm down to 105–150 cm. The soil texture varied among the layers from loamy sand, sandy loam, loam, to silty loam. These measured time-patterns of soil-water content were used by Braga (2000) in an optimization procedure by adaptive simulated annealing (Ingber, 1993) against values obtained by DSSAT simulations, to estimate the LL, DUL and SAT of each layer. We compared those optimized LL and DUL estimates with the estimates of each of the methods used here.

2.2.3. Step 3

The impact of the estimated LL, DUL and SAT on the simulated soybean yields was calculated with the CROPGRO-Soybean model (Boote et al., 1998) in DSSAT (Tsuji et al., 1994) for each of the texture combinations of step 1. Runs were done under water-limited conditions, but without *N* limitation (thus giving the water-limited potential yield), using 11 years of weather data (1986–1996) for Tifton, Georgia (USA). An existing Georgia soil file was used, in which texture, LL, DUL, SAT, K_{sat}, BD, and organic carbon were replaced by the combinations of step 1. A given soil texture combination was applied to all soil layers, thus giving a totally homogeneous profile in terms of texture, BD and hydraulic parameters. The soil depth (178 cm), nitrogen concentrations (data not available), pH (6.5), root distribution parameters, albedo (0.13), and runoff curve number (74.0) stayed at their original values. This was a purely academic exercise, as such soils may not exist at all in Georgia, but it gives a good impression of which soil type will give the biggest differences in crop yields with the different PTF methods. This resulted in over 5000 different texture combinations, to be run with 8 estimation methods for 11 years. Only those texture combinations that were allowed with a given method were included in the analysis. Planting dates were always the same (day of year 166 or 15 June), independent of soil texture

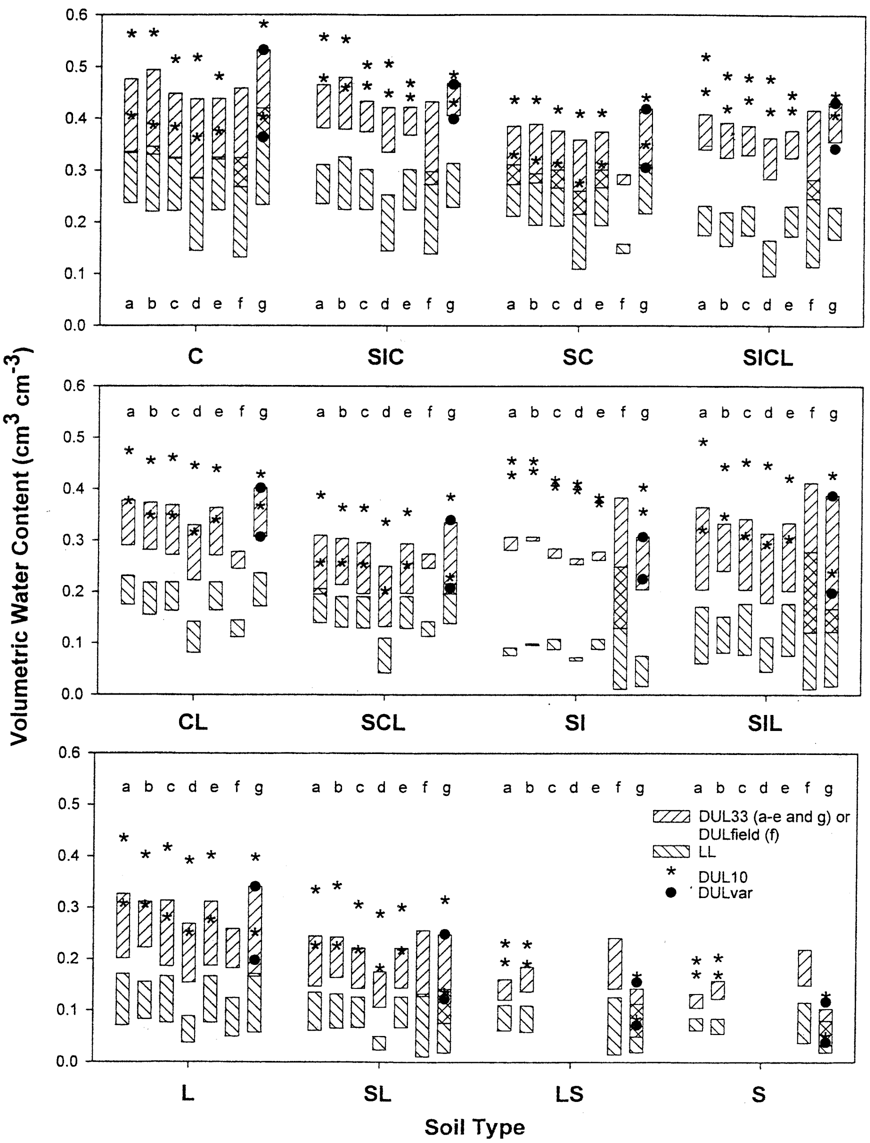

Fig. 1. Range of volumetric water content values obtained for the lower limit (LL) and drained upper limit (DUL) for 7 methods (letters a–g) for estimating the soil-water retention. The DUL was calculated at −33 kPa (DUL33, bar) and at −10 kPa (DUL10, asterisk); for the Method_Baumer–Rice, DUL was also calculated with a variable matric potential (DULvar, circle). Method_Ritchie1999 used field-measured data, which do not relate to matric potential (DULfield, bar). Methods used: a = Method_Rawls, b = Method_Saxton, c = Method_Rawls–Brakensiek with Brooks and Corey (1964), d = Method_Rawls–Brakensiek with Campbell (1974), e = Method_Rawls–Brakensiek (1985) with Van Genuchten (1980), f = Method_Ritchie1999, g = Method_Baumer–Rice. For the soil types, see Nomenclature in the Introduction.

and weather, so that differences in planting date did not affect the yield.

A common value of the saturated hydraulic conductivity (K_{sat}) was used for all water retention methods; it of course differed by soil type of each layer. Some authors also presented an equation for K_{sat} (e.g. Ritchie and Crum, 1989; Saxton et al., 1986), but others did not (e.g. Ritchie et al., 1999).

Using different K_{sat} equations for different water retention methods would compromise a ‘clean’ comparison of the water retention methods in the crop model runs. Therefore, the K_{sat} estimate according to Table 2 of Rawls et al. (1982) was used for all methods.

2.3. Statistics

For comparison of the difference between estimated water retention parameters and field-measured values, the mean absolute error ($MAE = 1/N\Sigma_{i=1}^{N}|P_i - O_i|$), root mean square error $RMSE = [1/N\Sigma_{i=1}^{N}(P_i - O_i)^2]^{0.5}$ and the index of agreement ($d = 1 - [\Sigma_{i=1}^{N}(P_i - O_i)^2/\Sigma_{i=1}^{N}(|P'_i| + |O'_i|)^2]$) were computed (Willmott, 1982); in these equations, P_i and O_i are, respectively, the predicted and observed values, N is the number of cases and $P'_i = P_i - \bar{O}$ and $O'_i = O_i - \bar{O}$. Willmott (1982) described MAE and RMSE as ‘among the best overall measures of model performance’, of which RMSE is more sensitive to extreme values due to its exponentiation; it therefore can be considered as a high estimate of the actual average error. The index of agreement (Willmott, 1981) is a standardized measure (scale 0–1) of the degree to which a model’s predictions are error free.

3. A critical note

Several of the methods compared in this paper show a worrisome lack of accuracy, either in their equation structure or in the presentation of the method in the article (Table 2). A number of errors were detected (see below: Method_Ritchie1987), several articles had typo’s in the equations (Method_Rawls and Method_Saxton), while sometimes elsewhere in the article the same equation was presented in correct form (Method_Saxton) and sometimes a method had been published several times but with slightly different equations (Method_Ritchie1987, Method_Baumer–Rice) or with a different level of precision (Method_Rawls–Brakensiek). This means that among the many methods available it is very difficult to identify how exactly a specific method was meant to be applied. This also may mean that many researchers have been using incorrect methods (we ourselves being among those people). Finally, if the FORTRAN code was available from the author, it sometimes deviated from the published version (Method_Baumer–Rice); although this may not be an error, because the code may have been updated after the article was published, it sometimes is difficult to know which version to use.

(A) Ritchie et al. (1987)—which also has been published as Ritchie et al. (1990) and as Ritchie and Crum (1989) and, with slightly different equations, as Ritchie et al. 1986—had several inaccuracies in the equations.

(i) If the BD is unknown, it is calculated by weighting the mineral fraction and the SOM fraction, each with its own BD. The equation applied for this, is, however, incorrect and does not work out in units. It should be: BD = 100/(SOM%/0.224 + (100–SOM%)/(mineral BD) (Adams, 1973; Rawls and Brakensiek, 1985).

(ii) Ritchie and Crum (1989) and Ritchie et al. (1990) state in the text that DUL increases by 17 volume percent per percent increase in BD. But in the equation, a factor of 197 is used, which makes the DUL explode with even a minor change in BD. The correct equation is used only in Ritchie et al. (1987).

(iii) First the BD, LL and DUL are calculated from the mineral soil fraction only and then corrections are applied for the effect of SOM. DUL is increased by 0.23 volume percent for each percent of SOM and the plant-extractable soil water is increased by 0.55 volume percent. But since the latter is defined as the difference between DUL and LL, this means that LL has to decline by 0.32 volume percent, which seems not what was meant (cf. Ritchie et al., 1999, who increase DUL by $0.01 \times C_{org}$ and the plant-extractable water content by $0.005 \times C_{org}$ meaning that LL increases by $0.005 \times C_{org}$).

(iv) Ritchie et al. (1986) give mostly the same equations as Ritchie et al. (1987, 1990) and Ritchie and Crum (1989), but they deviate at some points. These variations are not explained in any of the articles.

We corrected the ‘197’ error, as this was an obvious typo. But correcting the BD equation resulted in water contents reaching unlikely values

Table 2
Errors and inconsistencies found in the various water retention methods

Present equation	Corrected equation (as used by us)	Comment
Rawls et al. (1982)		
$\Theta = a + b$*sand$+c$*silt dd*clay$+c$*OM$+\cdots$	$\Theta = a + b$*sand$+c$*silt$+d$*clay$+e$*OM$+\cdots$	Regression equation (footnote to Table 3); in the Table 'e' does not exist and 'd' appears twice.
$\Theta = 0.7899 - 0.0037$*sand$+0.01$*OM-0.1315*BD. As a proxy for SAT	SAT = 0.95*POR	Though SAT is not given by the authors, the Θ at -4 kPa is close to it, but then SAT > POR for several texture combinations. Therefore SAT = 0.95*POR was used.
Rawls and Brakensiek (1985)		
$K_s = e$[19.52348*POR$-\ldots$20.019492*PC**2+ 0.0000173*PS**2*PC+0.02733*PC**2*POR+ 30.001434*PS**2*POR$-$0.0000035*PC**2*PS]	$K_s = e$[19.52348*POR$-\ldots$0.019492*PC**2+ 0.0000173*PS**2*PC+0.02733*PC**2*POR+ 0.001434*PS**2*POR$-$0.0000035*PC**2*PS]	The initial '2' and '3' are line-continuation symbols, but non-programmers may not recognize this. Such code specificities do not belong in an article.
Rawls and Brakensiek (1985), Rawls and Brakensiek (1989)		
Use the porosity instead of the saturated water content in the equations Brooks and Corey (1964), Campbell (1974) and Van Genuchten (1980).	Could not be fixed.	Correct equation in Rawls et al. (1991)
Rawls et al. (1991)		
Same equations as Rawls and Brakensiek (1985) but with less decimals, which just one example: $h_b = e[5.340 + \cdots + 0.00000(C^2)(S) + 0.500(\phi^2)(C)]$	$h = e[5.3396738 + \cdots + 0.0000054(C^2)(S) + 0.50028060(\phi^2)(C)]$	The corrected equation is from Rawls and Brakensiek (1985). The different # of decimals not only results in less accuracy but also in e.g. a multiplication by zero.
$\frac{\theta - \theta_r}{\theta_s - \theta} = (\frac{1}{1 + (\alpha h)^n})^m$	$\frac{\theta - \theta_r}{\theta_s - \theta_r} = (\frac{1}{1 + (\alpha h)^n})^m$	Table 1: the denominator of the equation of Van Genuchten (1980) uses θ_r and not θ.
Saxton et al. (1986)		
$B = e + f(\%C)^2 + g(\%S)^2 + g(\%S)^2(\%C)$	$B = e + f(\%C)^2 + g(\%S)^2(\%C)$	Table 2 has wrong equation; text has the correct one.
$\theta_s = 0.332 - 7.251*10^{-4}(\%\text{sand}) + 0.1276\log_{10}(\%\text{clay})$	SAT = 0.95*POR	SAT > POR for several texture combinations
Baumer and Rice (1988)		
Some soils are not classified correctly.	Critical limits adapted.	MUUF program comes with subroutine to classify the soils, but this does not cover all the texture combinations, so that some soils are classified incorrectly.
Ritchie and Crum (1989), Ritchie et al. (1990)		
$DUL_c = DUL_m - 197*(D_m - D_r) + 0.23*OM_f$	$DUL = DUL_m - 17*(D_m - D_f + 0.23*OM_f$	Correct in the text, wrong in the equation. Correct in equation of Ritchie et al. (1987)
$D_f = [OM_f*0.224 + (100 - OM_f)*D_m]/100$	$D_r = 100/[OM/0.224 + (100 - OM)/D_m$	Conversion from mineral BD to field BD. Gives BD > BDM with Ritchie's BDM. Correct equation from Adams (1973) and BDM from Rawls and Brakensiek (1985)
Ritchie et al. (1987)		

Table 2 (*Continued*)

Present equation	Corrected equation (as used by us)	Comment
$D_{mf} = (OM_f^* D_f - OM^*0.224)/(100 - OM)$	$D_{mf} = (100 - OM_f)/(100/BD - OM_f/0.224)$	Similar as D_r equation in Ritchie and Crum (1989) and Ritchie et al. (1990), but conversion in the opposite direction (field BD to mineral BD). Is given correctly in Ritchie et al. (1986), but with SOM as fraction and not%.
Ritchie and Crum (1989), Ritchie et al. (1987), Ritchie et al. (1990)		
$PLEXW_c = PLEXW_m + 3.5^*(D_m - D_f) + 0.55^*OM_f$	Not corrected.	PLEX equals DUL-LL, but if DUL increasesby 0.23 with OM and PLEXW by 0.55, then LL goes down by 0.32*OM.
Ritchie et al. (1986)		
W1 = 0.19 − 0.0017*SAN(I) sand > 75%	$LOL_m = 18.8 - 0.168^*SAND$	Though variable names units (% or $cm^3\ cm^{-3}$) differ from Ritchie and Crum (1989) equations mean the same. However, the coefficients in the equations are slightly different. Ritchie et al. (1987), Ritchie and Crum (1989) and Ritchie et al. (1990) apply 0.23 to DUL and 0.55 to plant-extractable water PLEXW, implying that LL goes down by 0.32*OM.
W1 = 0.16 silt > 70%	$LOL_m = 5.0 + 0.0244^*clay^2$	
W1 = 0.0542 + 0.00409*CLA(I) other soils	$LOL_m = 3.62 + 0.444^*clay$	
W2 = 0.429 − 0.00388*SAN(I) sand > 75%	$PLEXW_m = 0.423 - 0.00381^*sand$	
W2 = 0.1079 + 0.000504*SIL(I) silt > 70% and other soils	$PLEXW_m = 0.1079 + 0.0005004^*SIL(I)$	
LL = WI*(1 − XZ)*(1 + BDM(I) − BD(I) + 0.23*XZ	$LOL_c = DUL - PLEXW$	Ritchie et al. (1987), Ritchie and Crum (1989) and Ritchie et al. (1990) use in the text 17% (0.17) instead of 0.2, though in the equation it was 197% (not for Ritchie et al., (1987).
DUL(I) = LL(I) + W2*(1 − XZ) − (BDM(I) − BD(I))*0.2 + 0.55*XZ	$DUL_c = DUL_m - 197^*(D_m - D_f) + 0.23^*OM_f$	
	$PLEXW_c = PLEXW_m + 3.5^*(D_m - D_f)$	

BD, BDM = respectively, BD and BD of mineral particles (g cm^3); D_f, D_m, D_{mf}, respectively, field BD (with organic matter), and mineral BD (without organic matter) and mineral BD as calculated from field BD. DUL_c, DUL_m = DUL on the basis of respectively a ‘true’ soil (i.e. with organic matter and measured are calculated BD), and of mineral particles only. h = capillary suction; LOL_c, LOL_m = LL on the basis of respectively, a ‘true’ soil (i.e. with organic matter and measured or calculated BD), and of mineral particles only. OM, OM_f, OM% XZ = (field-measured) organic matter (%; in Ritchie et al., 1986) units are ‘fraction’. $PLEXW_c$,$PLEXW_m$ = plant-extractable water (%) on the basis of, respectively, a ‘true’ soil (i.e. with organic matter and measured or calculated BD), and of mineral particles only. PC, %C, C, CLA, Clay = percentage clay; POR = porosity (fraction) PS, %S, S, SAN, sand = percentage sand; SAT_E = effective saturation. SIL = percentage Slit; W2 = plant-extractable water (%) on the basis of mineral particles only. XZ = (field-measured) organic matter (%); α, n, m = constants; $\theta, \theta_r, \theta_n$ = volumetric water content, residual water content and saturated water content ($cm^3\ cm^{-3}$).

(e.g. DUL > SAT for most soils and DUL > 0.40 cm^3 cm^{-3} for a sandy soil). Apparently, the equations had been derived with at least some of the incorrect parameters or equations. The code may still be used if measured BD data are available (and the erroneous BD equation can be skipped), though it is not known whether other equations were affected by the error. For Figs. 3–5, we only used data that had a measured BD, and results were plausible.

(B) Rawls and Brakensiek (1985) presented their method with regression equations having up to eight decimals, but Rawls et al. (1991) presented the same equations with only three decimals for most factors; only some that have more than three decimal zero's are presented with four or five decimals, though there is also one that has a factor multiplied by 0.0000 while in the original article it is 0.0000054. This difference in significant digits has an important impact on the outcome.

(C) Rawls et al. (1982) presented in their Table 3 the regression coefficients to be used in an equation mentioned in a footnote to the table. In the table, one of the coefficients (*d*) is incorrectly named and the equation has two errors.

(D) Saxton et al. (1986) presented their equations in Table 2 and also in the text below Table 2, but one of the equations in the table is incorrect (confirmed by Saxton, personal communication).

(E) Baumer (1992) said that the organic carbon content of a soil is 1.7 times its SOM content, while it is the other way around (SOM $\approx 1.72 \times C_{org}$). How this affected the model equations is unknown.

(F) With the Baumer–Rice method, the soil needs to be categorized in the USDA soil classification system, for which the code provides a utility. This, however, does not cover all the possible texture combinations, so some soils were classified incorrectly; we corrected this in the code.

(G) The FORTRAN code for the Baumer–Rice method is available on the internet, as part of the MUUF model (Section 2). This code differs at several points from the original article of Baumer and Rice (1988) and from the MUUF users manual (Baumer et al., 1994). As pointed out above, this cannot be considered an error, as the code may be a more recent update. It is, however, confusing to the user.

(H) Rawls and Brakensiek (1985, 1989) and Rawls et al. (1991) used porosity in the equations of Brooks and Corey (1964), Campbell (1974), Van Genuchten (1980), though in the original articles, saturated water content was used. But citing from the manual of the RETC code for quantifying hydraulic functions of unsaturated soils (Van Genuchten et al., 1991, p. 5): 'the saturated water content should not be equated to the porosity of soils: θ_s of field soils is generally about 5–10% smaller than the porosity because of entrapped or dissolved air'. In Rawls and Brakensiek (1989), the entrapped air is calculated, but, surprisingly, it is not used with these equations. In the 1985 article, the porosity is indicated by $\phi = Q$ next to the equations (with Q = saturated porosity), which yet suggests that the saturated water content should be used. There is no explanation why this approach deviates from the original equations. This easily leads to errors, as scientists who are familiar with these equations may replace ϕ by θ_s or by the effective SAT, which is also presented in the table. Rawls (personal communication) confirmed that the parameters in his method had been estimated with the porosity and not with the saturated water content, and thus they should be used with porosity.

4. Results and discussion on step 1: method comparison across all texture combination

No results from the Method_Ritchie1987 are shown for the analyses described in step 1 and 3 of the materials and methods, because several errors were encountered in the equations, which had a major impact on the results. Some of these errors could be repaired in our code, but not all. As this method has been so widely used in crop modeling, we still show its application with Ritchie's original field-measured data (Figs. 3–5 and Tables 3–5). It is noteworthy though that this method gave quite a good agreement with field-measured values; this may point to a way for developing an improved method.

5. LL and DUL

Stepping through the texture triangle with steps of 1% clay and 1% sand, gave >5000 texture combinations covering the full range of soil types. As each soil type in the US soil classification involves many texture combinations, there will not be only one LL and DUL for a specific soil type, but a range of values of soil-water content, depending on the precise texture (Fig. 1). The primary focus for DUL was on the value at a water potential of −33 kPa (DUL33), but the −10 kPa value (DUL10; asterisk) is also indicated for those methods that allow it to be calculated.

The Method_Baumer–Rice makes a gradual transition between coarse- and fine-textured soils by considering several sand subclasses, giving a DUL at a matric potential that varies by texture. This variable-potential DUL is also identified (DULvar; circle). Method_Ritchie1987 and Method_Ritchie1999 base their estimate on field-measured DUL, not related to any matric potential (indicated as DULfield).

The range from the lower to upper bounds of LL and DUL33 (or DULfield) was quite large for most soil types, and in several cases the upper bound of LL overlapped with the lower bound of DUL33 (or DULfield). This overlap would not happen for a specific texture combination, however. For soil-type abbreviations like C, SI, LS, and S (see Nomenclature in the Introduction), many of the texture combinations did not result in estimates for some methods, as Method_Rawls, Method_Saxton, and Method_Rawls–Brakensiek exclude certain texture combinations. This may explain why SI, LS and S have relatively tight LL and DUL33 assemblies or no data at all, although it also reflects that some of these soil types do not cover a wide texture range.

DUL10 resulted often in a rather high water content, which was very different from DUL33. The range from its minimum to maximum value may be largely or completely above the range for DUL33 (e.g. SIC, CL, SICL, SI soils; Fig. 1). This ambiguity about which value to use for DUL is based on the assumption that field capacity would be lower (i.e. less negative) in a coarse-textured soil than in a fine-textured soil. The Method_Baumer–Rice uses a matric potential for DULvar that varies between −10.2 and −46 kPa, resulting in a θ range that for some soils was close to DUL33 (e.g. SC, CL), but for others approached DUL10 (e.g. LS, S). For SIC and SICL soils, the DULvar was calculated at, respectively, −44 and −46 kPa, resulting in DULvar values that was lower than the value for DUL33.

The computed saturated water content (SAT; not shown) varied considerably among methods. Ritchie et al. (1987) did not specify SAT, but Ritchie and Crum (1989), Ritchie et al. (1990) set SAT to 85% of the porosity. Method_Ritchie1999 set it equal to the porosity (in their SWLIMITS program, the article does not give SAT). Method_Rawls did not give SAT, but the SAT computed by the Method_Saxton resulted in values greater than the porosity. Method_Rawls–Brakensiek did not specify the relation between SAT and porosity, but the article suggests that they set SAT equal to porosity. The Method_Baumer–Rice estimated SAT values of up to 0.614 $cm^3\ cm^{-3}$ for clayey soils, which seems quite high. These high values relate to the high porosity this method estimated for clay soils (up to 0.678 $cm^3\ cm^{-3}$), due to the fact that it takes into account the clay activity as an attribute of expanding clays: the porosity calculated with the Method_Baumer–Rice was greater than the theoretical porosity as calculated from $POR = 1 - BD/APD$ (in which APD is the adjusted particle density, i.e. corrected for SOM). This high porosity also explains why for clayey soils (particularly C, SC and SCL) the calculated LL, DUL33 and DUL10 values were higher than for the other methods (Fig. 1). For the calculations in the rest of the article, we set SAT to 95% of the porosity (Van Genuchten et al., 1991, estimated 5–10% entrapped air). However, for the Method_Baumer–Rice we did not change the SAT equation, as this method may be meant specifically for expanding-clay soils; moreover the high POR value of the Method_Baumer–Rice not only affects SAT, but also LL and DUL.

5.1. Plant-extractable water

Subtracting LL from DUL gives the plant-extractable water content of the soil (often called

Table 3
Statistical analysis of the field capacity (DUL) estimates by eight methods

Soil	#obs.[a]	Error	DUL10						DUL33						DULvar	DUL field	
			Method_Rawls	Method_Saxton	Method_R–Br.+Brooks–C.	Method_R–Br. +Campbell	Method_R–Br.+Van G	Method_Baumer–Rice	Method_Rawls	Method_Saxton	Method_R–Br.+Brooks–C.	Method_R–Br.+Campbell	Method_R–Br.+Van G.	Method_Baumer–Rice	Method_Baumer–Rice	Method_Ritchie1999	Method_Ritchie1987
C	3	MAE	0.156	0.133	0.096	0.096	0.064	0.090	0.074	0.067	0.039	0.023	0.030	0.085	0.085	0.016	0.037
		RMSE	0.156	0.134	0.096	0.096	0.064	0.090	0.075	0.071	0.040	0.027	0.031	0.085	0.085	0.018	0.038
		d	0.256	0.306	0.364	0.372	0.479	0.361	0.473	0.516	0.671	0.807	0.745	0.382	0.382	0.881	0.643
SIC	17/9	MAE	0.141	0.115	0.084	0.085	0.055	0.071	0.052	0.044	0.036	0.029	0.033	0.068	0.067	0.041	0.053
		RMSE	0.146	0.120	0.096	0.096	0.068	0.087	0.063	0.056	0.046	0.037	0.043	0.084	0.083	0.047	0.066
		d	0.225	0.251	0.234	0.246	0.203	0.486	0.369	0.357	0.155	0.484	0.118	0.491	0.489	0.754	0.195
SICL	47/36	MAE	0.141	0.100	0.090	0.087	0.055	0.078	0.047	0.035	0.030	0.030	0.029	0.060	0.054	0.039	0.028
		RMSE	0.148	0.106	0.099	0.096	0.067	0.086	0.059	0.039	0.038	0.038	0.036	0.070	0.065	0.044	0.034
		d	0.261	0.327	0.326	0.330	0.390	0.348	0.425	0.463	0.357	0.308	0.283	0.376	0.383	0.274	0.615
CL	37	MAE	0.119	0.085	0.082	0.067	0.067	0.091	0.046	0.043	0.041	0.048	0.041	0.066	0.066	0.053	0.043
		RMSE	0.128	0.099	0.096	0.083	0.080	0.101	0.058	0.052	0.049	0.056	0.048	0.078	0.078	0.060	0.052
		d	0.391	0.428	0.434	0.464	0.462	0.422	0.564	0.477	0.480	0.475	0.470	0.480	0.480	0.328	0.387
SCL	13	MAE	0.037	0.022	0.028	0.041	0.025	0.043	0.045	0.040	0.055	0.112	0.056	0.024	0.025	0.046	0.043
		RMSE	0.041	0.025	0.034	0.055	0.033	0.048	0.055	0.045	0.062	0.117	0.063	0.033	0.032	0.047	0.044
		d	0.320	0.477	0.412	0.274	0.417	0.217	0.275	0.306	0.241	0.134	0.238	0.432	0.440	0.230	0.284
SL	1/0	MAE	*	*	*	*	*	0.064	*	*	*	*	*	0.020	0.020	0.008	0.107
		RMSE	*	*	*	*	*	0.064	*	*	*	*	*	0.020	0.020	0.008	0.107
		d	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*
SIL	74/48	MAE	0.196	0.154	0.161	0.146	0.134	0.106	0.085	0.067	0.069	0.048	0.067	0.063	0.063	0.029	0.043
		RMSE	0.200	0.162	0.169	0.154	0.146	0.123	0.091	0.073	0.074	0.052	0.071	0.078	0.078	0.037	0.051
		d	0.187	0.193	0.189	0.208	0.185	0.493	0.295	0.236	0.318	0.681	0.322	0.603	0.603	0.908	0.730
L	40	MAE	0.110	0.091	0.074	0.051	0.062	0.101	0.028	0.029	0.028	0.048	0.028	0.038	0.038	0.022	0.026
		RMSE	0.115	0.099	0.082	0.062	0.073	0.106	0.037	0.040	0.034	0.056	0.034	0.046	0.046	0.031	0.034
		d	0.401	0.423	0.479	0.550	0.495	0.704	0.719	0.635	0.772	0.626	0.763	0.804	0.704	0.804	0.800
SL	10/9	MAE	0.078	0.048	0.039	0.029	0.039	0.069	0.034	0.025	0.036	0.089	0.037	0.027	0.033	0.024	0.019
		RMSE	0.087	0.056	0.042	0.039	0.042	0.076	0.039	0.030	0.050	0.095	0.050	0.031	0.035	0.030	0.023
		d	0.418	0.562	0.571	0.488	0.548	0.496	0.621	0.746	0.483	0.332	0.482	0.798	0.698	0.762	0.871
LS	1/0	MAE	0.063	0.058	*	*	*	0.043	0.002	0.014	*	*	*	0.005	0.009	0.061	0.013
		RMSE	0.063	0.058	*	*	*	0.043	0.002	0.014	*	*	*	0.005	0.009	0.061	0.013
		d	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*
S	29/1	MAE	0.074	0.086	*	*	*	0.010	0.018	0.050	*	*	*	0.022	0.013	0.094	0.024
		RMSE	0.074	0.086	*	*	*	0.012	0.018	0.050	*	*	*	0.025	0.015	0.095	0.029
		d	0.417	0.376	*	*	*	0.541	0.806	0.530	*	*	*	0.412	0.550	0.168	0.395

The field capacity was calculated at −10 kPa (DUL10), at −33 kPa (DUL33); and at a variable matric potential (DULvar; Method_Baumer–Rice); Method_Ritchie1987 and Method_Ritchie1989 do not use matric potential (DULfield). The estimated data were compared with a subset of the field-measured data of Ratliff et al. (1983), Ritchie et al. (1987). For the soil types, see Nomenclature in the Introduction. MAE, Mean Absolute Error; RMSE, Root Mean Square Error; d, Willmott's index of agreement. R. & Br., Rawls and Brakensiek; Van G., Van Genuchten; Brooks–C, Brooks–Corey.

[a] Method_Rawls, Method_Saxton and Method_Rawls–Brakensiek have limitations on the texture range they are applicable to and therefore could not be used with all soils available. The number on the left indicates the total number of soils and the number on the right indicates the soils that were used for these methods.

AWHC). In many crop models, plant-extractable water is more important than the precise values of DUL and LL. In agreement with the terminology used for DUL at different matric potentials, we use here also AWHC33, AWHC10, AWHCvar and AWHCfield for the AWHC calculated from DUL at, respectively, −33, −10 kPa, a variable matric potential (Method_Baumer–Rice) and from field-measured data (Method_Ritchie1987, Method_Ritchie1999).

The most notable difference between the methods is that Method_Ritchie1999 used a fundamentally different approach than all the other methods. It is based on the assumption that all soils, except the very sandy ones, have an almost identical plant-extractable water content of about 0.132 $cm^3 cm^{-3}$ using the equation $AWHC = 0.132 - 2.5 \times 10^{-6} \exp(0.105 \times sand) + 0.005 \times C_{org}$ (in which C_{org} is the organic carbon content).

Fig. 2 presents the range in AWHC for each soil type, calculated for the > 5000 textural combinations that cover the soil triangle (step 1 in Section 2, Materials and Methods). It shows that the AWHC varies greatly, not only between methods and soil types, but just as well within soil types. There generally is an uncertainty in AWHC of at least a 0.05 $cm^3 cm^{-3}$ if one only knows the soil type; exceptions are Method_Ritchie1999 for non-sandy soils (see above), Method_Rawls–Brakensiek with SIC, SC and SICL and all methods but Method_Baumer–Rice with SI. For some soils and methods, the uncertainty even reached 0.14 $cm^3 cm^{-3}$ (Method_Baumer–Rice for SL). Crop modelers who apply their model to a large area for which they have limited input data often need to make generalizing assumptions or simplifications. One of these could be to estimate soil-water-retention parameters according to soil type. Fig. 2 shows that for crop-modeling purposes this generalization would lead to large errors in input data, depending on the specific texture within the soil class. This result implies that the exact textural composition is needed for accurate representation of soils in a crop-modeling study.

The ambiguity among methods is worrisome for crop modelers. Given that a small difference in plant-extractable water content (e.g. 0.03 $cm^3 cm^{-3}$) can be enough to make the difference between a good yield and a poor yield in simulations, particularly on soils with a low AWHC and with limited rainfall. If soil parameters have been estimated using only soil-class information and any of the PTFs, it is not likely that model results would represent yields measured in a specific field having a soil in that texture class.

6. Results and discussion on step 2: method comparison using field-measured data

Fig. 3 shows the DUL33 (Method_Rawls, Method_Saxton, Method_Rawls–Brakensiek), DULvar (Method_Baumer–Rice) and DULfield (Method_Ritchie1987, Method_Ritchie1999) estimates, plotted against the field-measured data of Ritchie et al. (1987). The DUL10 estimates are not shown, as this would cloud the figure too much, but Table 3 shows the statistics of all estimates, classified by soil type. The DUL33 estimates of Method_Rawls and Method_Saxton were similar, which is not surprising, as these methods are based on the same dataset. The Method_Rawls–Brakensiek gave different results, depending on the follow-up method used: Brooks–Corey and Van Genuchten gave good agreement (Table 3: low MAE and RMSE; high d) with DUL33, but Campbell underestimated it for medium-textured soils (SCL and SL), DUL33 was in better agreement with the observed data than DUL10, except for sandy–clay–loam soils, for which DUL10 seemed more appropriate. One has to keep in mind that the methods of Method_Rawls, Method_Saxton and Method_Rawls–Brakensiek do not apply to very-coarse-textured soils, which are the ones for which DUL10 is generally thought of as being more appropriate. Because soils with > 70% sand had to be removed from the dataset for these methods, it is not unexpected that DUL10 always overestimated.

The two methods of Ritchie are based on field-measured DUL values and thus do not consider matric potential. The Ritchie methods are not independent of the data used for comparison, as the same dataset was used to derive them. Given the wide use of these methods (particularly Method_Ritchie1987) among crop modelers, we decided

Table 4
Statistical analysis of the wilting point LL estimates by eight methods

Soil type	#obs [a]	Error	Lower Limit							
			Method_Rawls	Method_Saxton	Method_R – Br. + Brooks – C.	Method_R – Br. + Camp-bell	Method_R – Br. + Van G.	Method_Baumer – Rice	Method_Ritchie1999	Method_Ritchie1987
C	3	MAE	0.051	0.042	0.043	0.050	0.043	0.039	0.039	0.035
		RMSE	0.063	0.066	0.059	0.051	0.059	0.051	0.041	0.042
		d	0.092	0.036	0.071	*	0.071	0.098	*	0.155
SIC	17/9	MAE	0.042	0.038	0.038	0.051	0.038	0.051	0.043	0.055
		RMSE	0.049	0.045	0.044	0.060	0.044	0.062	0.051	0.067
		d	0.320	0.455	0.422	0.688	0.422	0.217	0.728	0.360
SICL	47/36	MAE	0.028	0.029	0.025	0.069	0.025	0.028	0.042	0.029
		RMSE	0.037	0.042	0.036	0.078	0.035	0.041	0.049	0.039
		d	0.349	0.454	0.404	0.358	0.408	0.424	0.242	0.644
CL	37	MAE	0.040	0.038	0.039	0.072	0.039	0.039	0.055	0.043
		RMSE	0.052	0.047	0.048	0.084	0.048	0.050	0.067	0.052
		d	0.453	0.422	0.408	0.467	0.408	0.426	0.432	0.426
SCL	13	MAE	0.055	0.062	0.064	0.149	0.064	0.050	0.094	0.082
		RMSE	0.060	0.066	0.068	0.151	0.068	0.056	0.096	0.084
		d	0.337	0.326	0.320	0.176	0.320	0.361	0.239	0.271
SI	1/0	MAE	*	*	*	*	*	0.106	0.018	0.123
		RMSE	*	*	*	*	*	0.106	0.018	0.123
		d	*	*	*	*	*	*	*	*
SIL	74/48	MAE	0.038	0.026	0.039	0.030	0.039	0.045	0.029	0.032
		RMSE	0.043	0.031	0.042	0.040	0.042	0.057	0.036	0.045
		d	0.623	0.820	0.551	0.868	0.551	0.484	0.898	0.723
L	40	MAE	0.031	0.026	0.030	0.046	0.030	0.028	0.024	0.034
		RMSE	0.036	0.032	0.035	0.054	0.035	0.033	0.029	0.038
		d	0.652	0.643	0.654	0.517	0.654	0.762	0.762	0.700
SL	10/9	MAE	0.046	0.038	0.037	0.063	0.037	0.037	0.030	0.019
		RMSE	0.051	0.042	0.042	0.078	0.042	0.041	0.034	0.025
		d	0.487	0.564	0.526	0.421	0.526	0.619	0.747	0.905
LS	1/0	MAE	0.031	0.031	*	*	*	0.020	0.041	0.007
		RMSE	0.031	0.031	*	*	*	0.020	0.041	0.007
		d	*	*	*	*	*	*	*	*
S	29/1	MAE	0.051	0.055	*	*	*	0.008	0.080	0.028
		RMSE	0.051	0.055	*	*	*	0.012	0.081	0.035
		d	*	*	*	*	*	0.290	0.087	0.156

The estimated data were compared with a subset of the field-measured data of Ratliff et al. (1983) and Ritchie et al. (1987). For the soil types, see Nomenclature in the Introduction. MAE, Mean Absolute Error; RMSE, Root Mean Square Error; d, Willmott's index of agreement. R–Br., Rawls–Brakensiek; Van G., Van Genuchten; Brooks-C., Brooks–Corey.

[a] Method_Rawls, Method_Saxton and Method_Rawls–Brakensiek have limitations on the texture range they are applicable to and therefore could not be used with all soils available. The number on the left indicates the total number of soils and the number on the right indicates the soils that were used for these methods.

to yet include them. The remarkably good fit for Method_Ritchie1987, and less so for Method_Ritchie1999, is thus not surprising. Method_Baumer–Rice 1988 overestimated DUL with DULvar for most soils, but was among the best fitting methods for sandy and sandy–clay–loam soils (Table 3). DULvar was close to DUL10 for measured θs <0.15 (e.g. S), and approximated DUL33 for measured θs >0.30 (e.g. C, CL).

Fig. 4 shows the LL estimates and their field-measured equivalents. All methods resulted in a rather wide data cloud, showing a generally poor fit. Though the MAE and RMSE in Table 4 seen not bad compared to the DUL statistics of Table 3, one has to realize that the LL errors apply to much smaller estimated values than the DUL errors. An error of 0.05 on a LL of 0.03 cm^3 cm^{-3} (as for a sandy soil) means an error of almost 170%, while a DUL error of 0.10 on an estimated DUL of 0.30 cm^3 cm^{-3} is an error of about 30%. The Method_Rawls overestimated LL by up to 0.16 cm^3 cm^{-3} for measured θ values <0.15 and underestimated for high θ values. Saxton showed a similar pattern. The results of Method_Rawls–Brakensiek strongly depended on the follow-up method used: Brooks–Corey and Van Genuchten sometimes overestimated and other times underestimated, while Campbell always underestimated significantly except for very low θ values. The two Ritchie methods did not give a good fit with the measured data either, though Method_Ritchie1987 was quite good at low values of measured θ Method_Baumer–Rice gave a good fit for the low-θ part of the data, but veered off at intermediate θ values and underestimated at the high-θ end.

The estimated plant-extractable water content (Fig. 5) was calculated as AWHC = DUL−LL, using DUL33, DULvar (Baumer–Rice) and DULfield (Method_Ritchie1987, Method_Ritchie 1999); one can get an impression of what the difference would be with DUL10 from Fig. 1. Method_Rawls and Method_Saxton gave a cloud of AWHC values with a tendency to overestimate. They gave a low mean absolute error and RMSE values with AWHC33 for SCL, SL, L (Table 5), though the index of agreement was not very good for L. These methods also performed well for C and CL according to the index of agreement, but not as much according to the mean absolute error and RMSE. For other soils, the estimated AWHC deviated on average by at least 0.04 cm^3 cm^{-3} from the measured value. The Method_Rawls–Brakensiek gave a fair fit with Brooks–Corey and Van Genuchten for intermediate θ values, but underestimated significantly for high θ values. For SIC, SICL, SCL, CL, and L the mean absolute error was low (the RMSE a bit less so) and the index of agreement was high. With the Campbell follow-up method only loamy soils resulted with low error indicators. The Method_Ritchie1987 method estimated for most soils (besides the sandy ones) a rather narrow range of A WHCfield values (Fig. 5), though the field-measured data for these soils ranged from 0.06 to 0.23 cm^3 cm^{-3}. Yet, Method_Ritchie1987 did quite well in the statistics for all soils but SCL and especially well for S. Method_Ritchie1999 resulted in a low mean absolute error and RMSE for SIC, SICL, L, SL and S, though the index of agreement was good only for SIC and S. The Method_Baumer–Rice significantly overestimated AWHC for most soils, but gave a good mean absolute error, RMSE and index of agreement for S and SL. AWHCvar proved better than AWHC10 for the latter method, except for sandy soils, for which AWHC10 did better than AWHCvar. AWHCvar was close to AWHC33 for those soils where DULvar was almost the same as DUL33 (C, SIC, CL, SCL, SIL, L).

The Method_Rawls, Method_Saxton and Method_Rawls–Brakensiek do not apply to soils high in clay, very high in sand or very low in either sand or clay; for Method_Rawls–Brakensiek the allowable range is a bit tighter than for Method_Rawls and Method_Saxton. Consequently, many of the soils available could not be used for these methods: only 1 out of 29 was used for S, 0 out of 1 for LS (Method_Rawls–Brakensiek only; Method_Rawls and Method_Saxton used all), 9 out of 10 for SL (Method_Rawls–Brakensiek only), 0 out of 1 for SI, 48 out of 74 for SIL, 36 out of 47 for SICL and 9 out of 17 for SIC. Only Method_Ritchie1987 and Method_Ritchie1999 and Method_Baumer–Rice, apply to soils of any texture and thus dealt with very sandy soils in this

Table 5
Statistical analysis of the plant-extractable water content (available-water-holding capacity, AWHC) estimates by eight methods

Soil	#obs.[a]	Error	AWHC10						AWHC33						AWHC-var	AWHCfield	
			Method_Rawls	Method_Saxton	Method_R–Br.+Brooks–C.	Method_R–Br.+Campbell	Method_R–Br.+Van G.	Method_Baumer–Rice	Method_Rawls	Method_Saxton	Method_R–Br.+Brooks–C.	Method_R–Br.+Campbell	Method_R–Br.+Van G.	Method_Baumer–Rice	Method_Baumer–Rice	Method_Ritchie1999	Method_Ritchie1987
C	3	MAE	0.105	0.090	0.056	0.106	0.047	0.055	0.032	0.036	0.031	0.047	0.030	0.052	0.052	0.030	0.026
		RMSE	0.108	0.096	0.066	0.116	0.048	0.065	0.035	0.039	0.035	0.051	0.039	0.060	0.060	0.030	0.028
		d	0.335	0.341	0.313	0.248	0.031	0.317	0.556	0.480	0.028	0.292	0.239	0.331	0.331	0.277	0.237
SIC	17/9	MAE	0.129	0.113	0.074	0.132	0.042	0.068	0.040	0.041	0.025	0.050	0.025	0.065	0.062	0.023	0.023
		RMSE	0.131	0.116	0.080	0.136	0.049	0.073	0.047	0.050	0.030	0.058	0.028	0.070	0.067	0.028	0.028
		d	0.284	0.300	0.392	0.279	0.489	0.361	0.514	0.465	0.478	0.457	0.447	0.370	0.376	0.431	0.506
SICL	47/36	MAE	0.143	0.123	0.095	0.156	0.061	0.092	0.045	0.045	0.024	0.060	0.020	0.074	0.067	0.018	0.019
		RMSE	0.145	0.125	0.100	0.159	0.067	0.096	0.050	0.048	0.030	0.063	0.026	0.077	0.070	0.022	0.023
		d	0.151	0.167	0.192	0.137	0.239	0.253	0.321	0.314	0.331	0.273	0.340	0.303	0.326	0.273	0.446
CL	37	MAE	0.098	0.086	0.075	0.134	0.058	0.075	0.028	0.033	0.025	0.048	0.024	0.051	0.051	0.027	0.024
		RMSE	0.102	0.091	0.081	0.137	0.064	0.079	0.032	0.037	0.031	0.053	0.030	0.056	0.056	0.033	0.030
		d	0.338	0.341	0.376	0.264	0.428	0.389	0.581	0.446	0.417	0.437	0.409	0.439	0.439	0.377	0.389
SCL	13	MAE	0.076	0.069	0.063	0.108	0.059	0.087	0.016	0.024	0.018	0.037	0.017	0.042	0.047	0.049	0.039
		RMSE	0.078	0.071	0.067	0.111	0.063	0.089	0.019	0.027	0.020	0.042	0.020	0.046	0.050	0.050	0.042
		d	0.223	0.232	0.243	0.165	0.252	0.198	0.520	0.408	0.460	0.332	0.458	0.325	0.305	0.296	0.336
SI	1/0	MAE	*	*	*	*	*	0.170	*	*	*	*	*	0.086	0.086	0.009	0.015
		RMSE	*	*	*	*	*	0.170	*	*	*	*	*	0.086	0.086	0.009	0.015
		d	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*
SIL	74/48	MAE	0.167	0.143	0.129	0.176	0.103	0.122	0.052	0.047	0.034	0.055	0.033	0.072	0.073	0.026	0.027
		RMSE	0.170	0.148	0.134	0.179	0.110	0.127	0.058	0.055	0.040	0.060	0.039	0.078	0.078	0.033	0.031
		d	0.224	0.229	0.241	0.205	0.253	0.291	0.450	0.388	0.366	0.407	0.301	0.407	0.406	0.303	0.313
L	40	MAE	0.085	0.073	0.053	0.095	0.044	0.082	0.022	0.021	0.027	0.020	0.029	0.026	0.026	0.022	0.025
		RMSE	0.090	0.079	0.059	0.098	0.050	0.088	0.027	0.027	0.035	0.023	0.036	0.030	0.030	0.027	0.029
		d	0.305	0.320	0.377	0.298	0.382	0.454	0.259	0.197	0.516	0.595	0.502	0.258	0.454	0.258	0.320
SL	10/9	MAE	0.054	0.036	0.024	0.047	0.023	0.057	0.027	0.026	0.045	0.032	0.045	0.023	0.019	0.021	0.020
		RMSE	0.059	0.043	0.032	0.056	0.030	0.063	0.032	0.032	0.051	0.038	0.051	0.026	0.024	0.025	0.025
		d	0.412	0.431	0.442	0.416	0.435	0.404	0.505	0.425	0.390	0.360	0.393	0.323	0.346	0.391	0.363
LS	1/0	MAE	0.032	0.027	*	*	*	0.023	0.033	0.017	*	*	*	0.025	0.011	0.020	0.020
		RMSE	0.032	0.027	*	*	*	0.023	0.033	0.017	*	*	*	0.025	0.011	0.020	0.020
		d	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*
S	29/1	MAE	0.023	0.031	*	*	*	0.011	0.033	0.005	*	*	*	0.029	0.015	0.014	0.010
		RMSE	0.023	0.031	*	*	*	0.013	0.033	0.005	*	*	*	0.031	0.018	0.017	0.012
		d	*	*	*	*	*	0.505	*	*	*	*	*	0.347	0.504	0.506	0.539

The AWHC was calculated as θ at field capacity minus θ at wilting point, in which the field capacity was calculated at −10 kPa (AWHC10), at −33 kPa (AWHC33); and at a variable matric potential (AWHCvar; Method_Baumer–Rice); Method_Ritchie1987 and Method_Ritchie1999 do not relate it to a certain matric potential (AWHCfield). The estimated data were compared with a subset of the field-measured data of Ratliff et al. (1983) and Ritchie et al. (1987). For the soil types, see Nomenclature in the Introduction. MAE, Mean Absolute Error; RMSE, Root Mean Square Error; d, Willmott's index of agreement. R–Br., Rawls–Brakensiek; Van G., Van Genuchten; Brooks–C., Brooks–Corey.

[a] Method_Rawls, Method_Saxton and Method_Rawls–Brakensiek have limitations on the texture range they are applicable to and therefore could not be used with all soils available. The number on the left indicate the total number of soils and the number on the right indicates the soils that were used for these methods.

dataset. These three methods gave widely different water retention estimates for such soils (Table 6). LL values as low as 0.008 $cm^3 cm^{-3}$ and DUL values down to 0.068 $cm^3 cm^{-3}$ were measured for soils of over 95% sand. None of the methods dealt accurately with such soils, though Method_Ritchie1987 and Method_Baumer–Rice performed reasonably for soil #1–4 in Table 6, but not for soil #5; Method_Ritchie1999 did poorly with both LL and DULfield. Method_Baumer–Rice used a matric potential of 16.2 kPa for DULvar of these soils, which overestimated the measured value; with DUL10 this method performed better.

Since Method_Ritchie1987 and Method_Ritchie1999 were developed with the same dataset of field-measured data that we used, there was a need to also use an independent dataset, for which we drew upon data of Braga (2000). Analyzed by soil type, it showed that the Method_Saxton was superior with almost all the statistics for LL, DUL and AWHC of all four soil types (Table 7). Method_Rawls–Brakensiek did not apply to the loamy sand, while it performed poorly with the Campbell follow-up method in the other three soils, apart from the AWHC of loamy soils. This technique seems an interesting approach to be used instead of the labor-intensive and weather-dependent measurement of soil-water parameters under field conditions. However, possible drawbacks are that results may be crop-model dependent and, due to the non-uniqueness of the inverse problem, may bare limited resemblance to actual soil physical parameters (personal communication Wendy Graham—Univ. Florida).

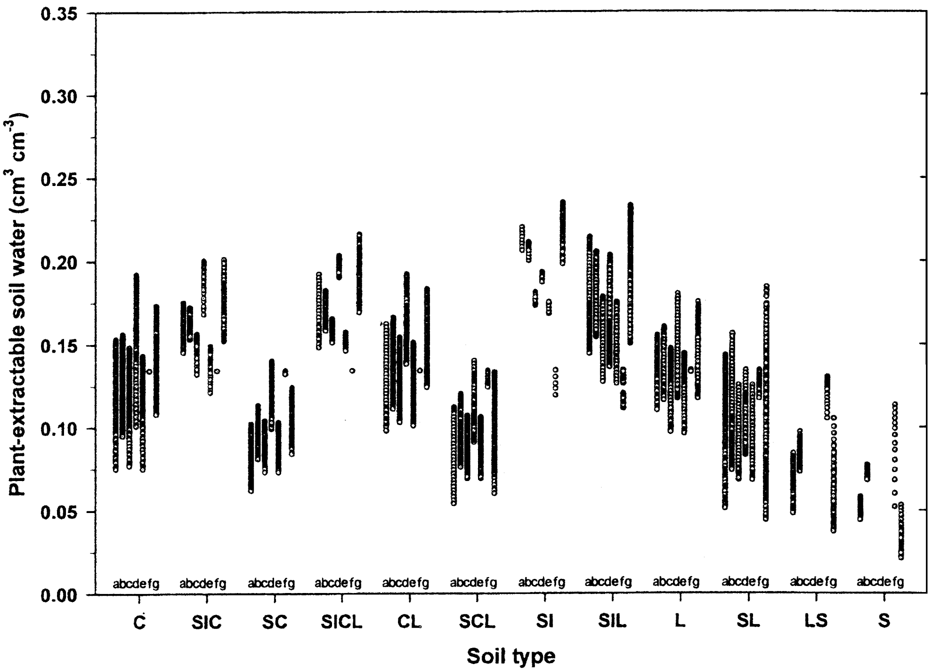

Fig. 2. Range of plant-extractable water content (also called 'available-water-holding capacity', AWHC), estimated as θ at field capacity (DUL) minus θ at wilting point (LL). Field Capacity (DUL) was calculated at −33 kPa (Method_Rawls, Method_Saxton, Method_Rawls–Brakensiek) or at a variable matric potential (Method_Baumer–Rice); Method_Ritchie1999 used field-measured data, which do not relate to matric potential. Seven methods for estimating the soil-water retention were applied (letters a–g; see the header of Fig. 1). The measured data were a subset of the field-measured data of Ratliff et al. (1983) and Ritchie et al. (1987). For the soil types, see Nomenclature in the Introduction.

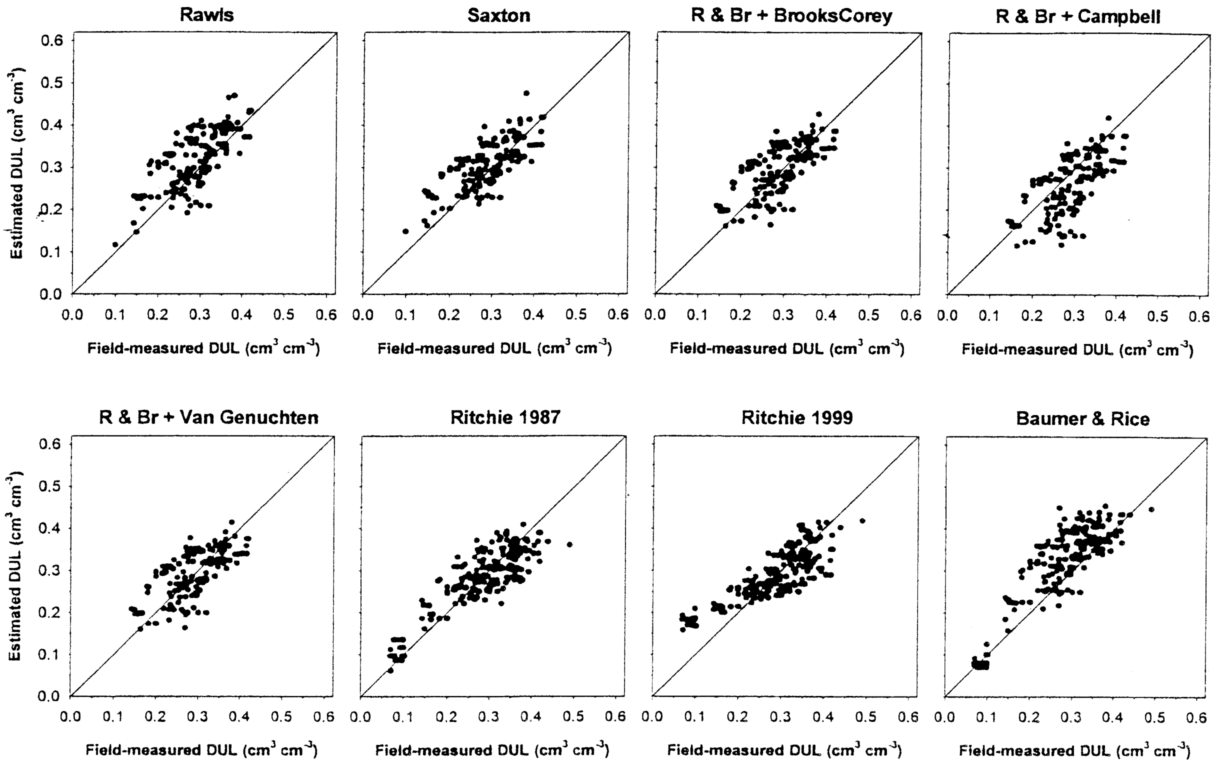

Fig. 3. Measured versus estimated volumetric water content at wilting point LL. Eight methods for estimating the soil-water retention were applied (see the header of Fig. 1). The measured data were a subset of the field-measured data of Ratliff et al. (1983), Ritchie et al. (1987).

Table 6
Measured and estimated wilting point LL and field capacity DUL of the three most-sandy soils in the dataset used, which is a subset of the field-measured data of Ratliff et al. (1983) and Ritchie et al. (1987)

	Field-measured		Method_Ritchie1987		Method_Ritchie1999		Method_Baumer–Rice			
	LL	DUL	LL	DULfield	LL	DULfield	LL	DUL10	DUL33	DULvar
Soil #1: 97.4% sand/1.7% clay	0.008	0.068	0.001	0.062	0.092	0.158	0.033	0.091	0.070	0.091
Soil #2: 96.2% sand/1.2% clay	0.031	0.101	0.036	0.097	0.093	0.167	0.030	0.101	0.073	0.100
Soil #3: 95.7% sand/2.8% clay[a]	0.019	0.068	0.037	0.097	0.106	0.183	0.033	0.089	0.068	0.080
	0.029	0.079	0.037	0.097	0.106	0.183	0.033	0.089	0.068	0.080
Soil #4: 95.1% sand/2.0% clay[a]	0.020	0.092	0.060	0.117	0.106	0.185	0.027	0.086	0.063	0.076
	0.024	0.094	0.060	0.117	0.108	0.186	0.029	0.090	0.066	0.080
Soil #5: 89.2% sand/7.7% clay	0.018	0.098	0.031	0.117	0.106	0.209	0.065	0.125	0.105	0.125

Field capacity was calculated at −33 kPa (DUL33), at −10 kPa (DUL10); and at a variable matric potential (DULvar) for Method_Baumer–Rice; Method_Ritchie1987 and Method_Ritchie1999 do not relate it to a certain matric potential (DULfield), as it is based on field-measured observations.

[a] Some pedons with an identical texture, SOM and BD, but positioned at a different depth, differ in LL or DUL; both are given here.

6.1. Other comparisons of water retention-estimation methods

Kern (1995) compared six methods—including those of Rawls et al. (1982), Saxton et al. (1986)—for estimating water retention at −10, −33 and −1500 kPa, based on lab-measured data. With Rawls and Saxton the statistics were more favorable for the −33 kPa values than for the −10 kPa values, but with other methods the opposite was found. All methods overestimated the water retention at −10 kPa for $\theta < 0.10$ cm^3 cm^{-3}, which presumably relates mostly to coarse-textured soils. Both Rawls and Saxton also overestimated water retention at −33 kPa for low θ values. Some of the methods gave a fair agreement for LL in the intermediate θ range, but deviated at low or high θ values. Timlin et al. (1996) compared the methods of Williams et al. (1992) and Rawls et al. (1992), the latter being identical to Rawls and Brakensiek (1985) used here. With Rawls, DUL10 gave a fair agreement at low and intermediate θ values, but overestimated at high θ values; DUL33 gave a fair agreement overall. The LL was underestimated for any θ value.

The method comparison in Kern and in Timlin show acceptable agreement between lab-measured data and estimated data for intermediate θ range, but the methods deviated at high and low θ values. Rawls et al. (1991; Table 7) show a difference in DUL as estimated by three methods of up to 0.08 and 0.06 cm^3 cm^{-3} for LL.

SOM is an important factor in defining a soil's water retention characteristics. Kern (1995) showed the impact of different SOM levels on water retention, as calculated with the method of Rawls et al. (1982). If the SOM level increases, a higher (more negative) matric potential is needed to obtain a specific volumetric water content. Often, however, the LL and DUL change in similar ways, so that the net effect on AWHC may be minor. Yet for big increases in SOM, the effect on AWHC cannot be ignored, as Kern showed an increase in AWHC of about 0.025 cm^3 cm^{-3}, with an increase 2% SOM. Saxton et al. (1986) derived their method with an average SOM concentration of 0.66%, which removed it from being a user-defined input; Rawls and Brakensiek (1985) do not use it either. The only effect of SOM on the water retention estimate with these methods is indirect through BD and porosity. Method_Saxton does not use BD or POR, but Method_Rawls–Brakensiek does use POR. If one has measured BD data, the conversion to POR becomes then important and should be done by using POR = 1 − BD/APD, in which the adjusted particle density APD has a SOM correction, instead of the commonly used POR = 1 − BD/2.65. Fixing the SOM content at a certain value, as was done in this method comparison, may lead to one not being able to discriminate well between methods that do use SOM as a factor in the equations (e.g. Method_Rawls) and those methods that do not (e.g. Method_Saxton). The latter do not seem adequate for use in soils with a SOM concentration that is considerably higher than 0.66%.

6.2. Comparison between lab- and field-measured data

Although the water retention parameters LL, DUL, SAT and AWHC do have a physical meaning, these parameters are not really precise physical hydrologic parameters, since they are soil-dependent (i.e. appropriate tension levels seem to depend on soil type), scale dependent (Diekkrüger, 1990), weather dependent (due to possible effects of hysteresis and antecedent moisture conditions) and crop dependent. Even if the parameters were true soil-physical parameters, they are extremely scale dependent (i.e. change with support volume of measurement) due to soil heterogeneity. These problems of model-dependent and scale-dependent parameters are widely recognized in hydrologic modeling, and are one of the impetuses behind stochastic modeling (Braud et al., 1995; Wu et al., 1997).

Most methods for estimating hydraulic parameters were based on lab-measured data, and only Ritchie et al. (1987, 1999) used field-measured data. These data covered seven soil orders, 60% of which were Mollisols and Alfisols (Ratliff et al., 1983), included all textural classes apart from sandy–clay and had very limited data in clay, loamy sand and silt. Obtaining field-measured data is far more complicated and labor intensive

Table 7
Mean absolute error (MAE) and root mean square error (RMSE) of estimated lower limit (LL), field capacity (DUL) and available-water-holding capacity (AWHC), versus measured-and-optimized data (Braga, 2000)

Soil type	#obs.	Parameter	error	Method_Rawls	Method_Saxton	Method_R–Br.+Brooks–Corey	Method_R–Br.+Campbell	Method_R–Br.+Van G.	Method_Baumer–Rice	Method_Richtie1999
LS	5	LL	MAE	0.014	0.014	*	*	*	0.030	0.014
			RMSE	0.015	0.018	*	*	*	0.034	0.015
			d	0.440	0.494	*	*	*	0.356	0.404
		DUL	MAE	0.029	0.011	*	*	*	0.057	0.048
			RMSE	0.031	0.017	*	*	*	0.060	0.050
			d	0.428	0.468	*	*	*	0.246	0.301
		AWHC	MAE	0.031	0.008	*	*	*	0.027	0.047
			RMSE	0.032	0.011	*	*	*	0.029	0.048
			d	0.381	0.567	*	*	*	0.393	0.269
SL	138	LL	MAE	0.009	0.005	0.005	0.072	0.005	0.009	0.012
			RMSE	0.011	0.009	0.007	0.073	0.007	0.012	0.013
			d	0.825	0.847	0.853	0.092	0.853	0.619	0.769
		DUL	MAE	0.032	0.006	0.035	0.086	0.035	0.014	0.037
			RMSE	0.035	0.011	0.036	0.087	0.036	0.019	0.040
			d	0.569	0.893	0.324	0.147	0.320	0.571	0.535
		AWHC	MAE	0.026	0.010	0.032	0.014	0.032	0.016	0.028
			RMSE	0.030	0.016	0.034	0.018	0.034	0.019	0.034
			d	0.449	0.575	0.342	0.505	0.339	0.418	0.427
L	158	LL	MAE	0.004	0.002	0.006	0.065	0.006	0.016	0.010
			RMSE	0.006	0.004	0.008	0.065	0.008	0.017	0.011
			d	0.940	0.964	0.892	0.222	0.892	0.571	0.806
		DUL	MAE	0.016	0.004	0.019	0.065	0.021	0.027	0.024
			RMSE	0.018	0.006	0.021	0.066	0.022	0.032	0.025
			d	0.832	0.965	0.792	0.384	0.774	0.485	0.705
		AWHC	MAE	0.016	0.005	0.024	0.007	0.026	0.013	0.015
			RMSE	0.017	0.008	0.026	0.009	0.027	0.017	0.016
			d	0.650	0.886	0.531	0.888	0.513	0.447	0.667
SIL	34	LL	MAE	0.006	0.002	0.017	0.052	0.017	0.028	0.016
			RMSE	0.007	0.003	0.017	0.052	0.017	0.029	0.016
			d	0.866	0.958	0.537	0.201	0.537	0.322	0.556
		DUL	MAE	0.013	0.008	0.009	0.049	0.011	0.071	0.040
			RMSE	0.016	0.012	0.013	0.050	0.015	0.072	0.042
			d	0.651	0.710	0.724	0.330	0.695	0.225	0.361
		AWHC	MAE	0.018	0.009	0.024	0.011	0.026	0.042	0.024
			RMSE	0.021	0.013	0.027	0.014	0.029	0.044	0.027
			d	0.486	0.522	0.436	0.465	0.417	0.302	0.413

Seven estimation methods were applied (see text). The AWHC was calculated as θ at field capacity minus θ at wilting point, in which the field capacity was calculated at −33 kPa (all methods but Method_Baumer–Rice), and at a variable matric potential (Method_Baumer–Rice); Method_Ritchie1999 does not relate it to a certain matric potential. MAE, Mean Absolute Error; RMSE, Root Mean Square Error; d, Willmott's index of agreement. R–Br., Rawls-Brakensick; Van G., Van Genuchten; Brooks–C., Brooks–Corey.

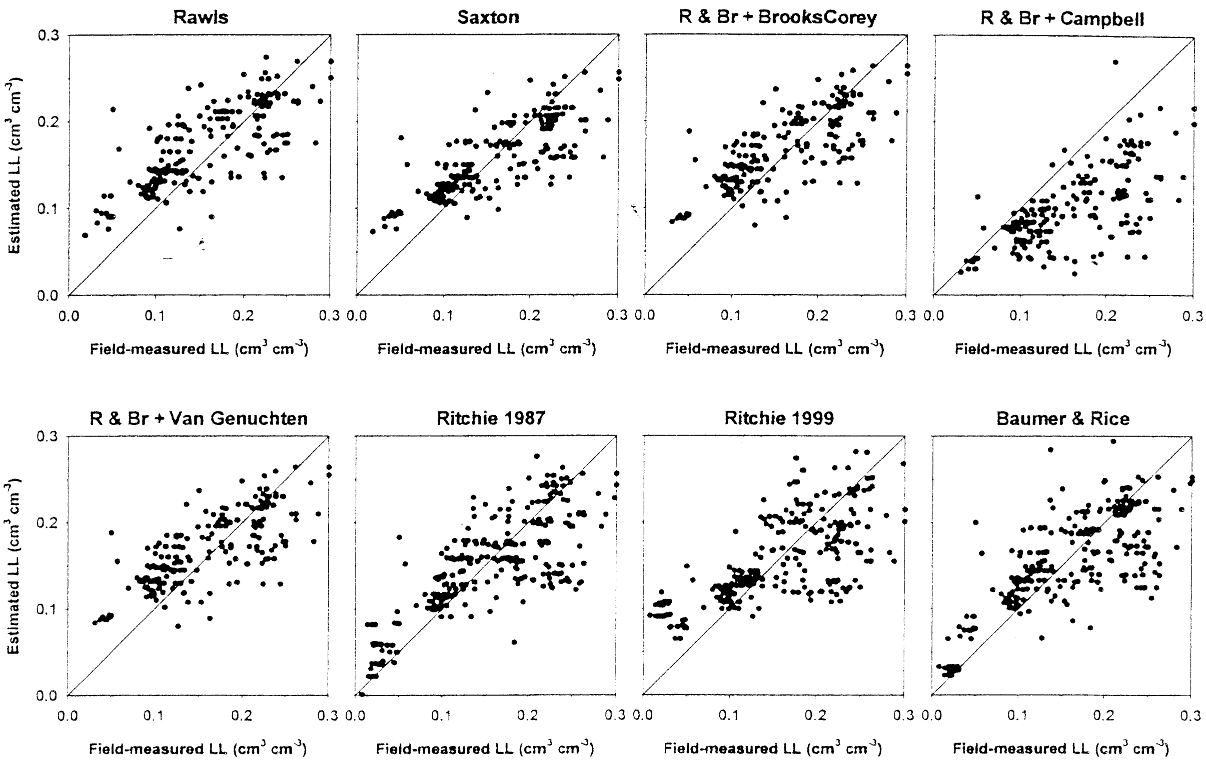

Fig. 4. Measured versus estimated volumetric water content at field capacity DUL. Eight methods for estimating the soil-water retention were applied (see the header of Fig. 1). Field capacity was calculated at −33 kPa (Method_Rawls, Method_Saxton, Method_Rawls_Brakensiek), at a variable matric potential (Method_Baumer–Rice) or from field-measured data, which do not relate to matric potential (Method_Ritchie1987, Method_Ritchie1999). The measured data were a subset of the field-measured data of Ratliff et al. (1983), Ritchie et al. (1987).

than obtaining lab-measured data. It needs the involvement of a great number of people at many locations—this was done in a joint effort of the Soil Conservation Service and the Agricultural Research Service of the USA—and is weather dependent. But once this is done, the data are representative of the reality crops experience and not of artificial laboratory conditions combined with a matric potential that researchers consider as ‘wilting point’ or ‘field capacity’. It is very disappointing therefore that the estimation method of Ritchie et al. (1987), which is based on this valuable dataset, has several errors.

Measuring water retention parameters under field conditions has it own specific complications which do not occur with lab measurements. For DUL measurements under field conditions, generally the soil is first wetted by either the wettest-soil-profile method, the ponded-water method, or the trickle-irrigation method, after which measurement is done by soil sampling or neutron probe. Wetting the soil completely and letting it drain till drainage ceases can be difficult with heavy clay soils where drainage is inherently slow and with shrink-swell soils where the water infiltration is slow, soil aggregates may slake and throttles may develop near the soil surface. Estimating LL under field conditions is difficult, because a soil layer may have reached LL while the plant may still survive by absorbing water from another layer that is wetter.

Ritchie et al. (1999) used these data for a new analysis and came up with a different set of equations than Ritchie et al. (1987). The authors assumed that the field-measured DUL was strongly correlated with the sand/clay ratio and formulated this as DUL $= 0.186 \times (\text{sand/clay})^{-0.14}$. The LL is calculated as the DUL minus the plant-extractable water, which is defined as a function of the sand content. Their approach has several limitations:

(1) The figure on DUL by weight versus the sand/clay ration (Fig. 1 in Ritchie et al., 1999) is on a log–log scale, which removes most of the data scatter. What looks like a rather tight relationship with little variation may not really be such a good relationship. This is also reflected in the poor fit at low $-\theta$ values in our Fig. 3. Moreover, a small change in the sand and clay content may give a big difference in their ratio and thus have a major impact on DULfield. For instance, a silt soil with 1% sand and 11% clay results in a DULfield of 0.383, while a silt soil with 19% sand and 1% clay gets a DUL of 0.129. This explains, the surprisingly wide range of DULfield estimates we found for silt soils with this method (Fig. 1).

(2) Though there is a rather wide cloud of data points in their graph of the soil's plant-extractable water content versus the sand content, the Method_Ritchie1999 method assumes that all soils, except the very sandy ones, have a comparable plant-extractable water content of about 0.132 $cm^3\ cm^{-3}$, based on their experience with field-measured data. Such a generalization is hard to defend.

(3) The authors did not set constraints on the applicability of the equations. This explains, for instance, the close DULfield and LL ranges for sandy clay and wide DULfield range for clay and silty soils (Fig. 1), as these soil types were hardly represented in the dataset.

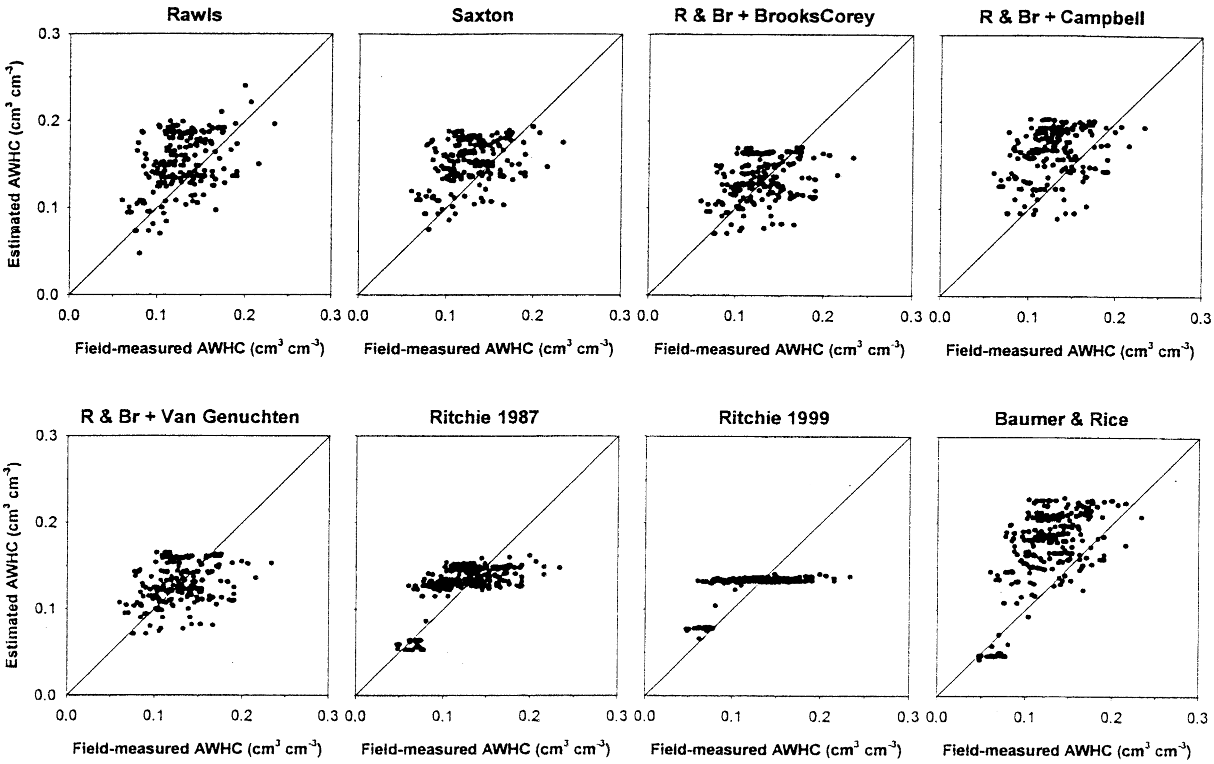

Fig. 5. Measured versus estimated plant-extractable water content AWHC, calculated as the difference between θ at field capacity and θ at wilting point. Eight methods for estimating the soil-water retention were applied (see the header of Fig. 1). Field capacity was calculated at −33 kPa (Method_Rawls, Method_Saxton, Method_Rawls–Brakensiek), at a variable matric potential (Method_Baumer–Rice) or from field-measured data, which do not relate to matric potential (Method_Ritchie1987, Method_Ritchie1999).

Besides determining field-measured water retention data, Ratliff et al. (1983) and Ritchie et al. (1987) also took soil samples from the same locations where the field-measurements were done, and sent these to a laboratory for determining LL (disturbed soil sample) and DUL (undisturbed soil core) with standard lab methods of, respectively, −1500 and −33 kPa. The results of this for the extract of the total dataset that we used are shown in Fig. 6. Clearly the lab-measured LL and DUL differ significantly from the field-measured data. Up to LLs of about 0.13 $cm^3 cm^{-3}$, the LL obtained in a lab is similar to that obtained in the field; above those values that lab-measured data increasingly underestimate what is measured in the field. Ratliff et al. (1983) stated that the lab-measured LL overestimated for L, SIC, C and underestimated for S, SIL, SCL. The data used here show an overestimation for L, CL, SL, SIL and an underestimation for SIL, SCL, SICL and CL. The lab-measured data significantly underestimated DUL for most samples compared to the field-measured data, meaning that the field capacity that plants experience is a lot wetter than what is characterized in the lab as 'field capacity'. This discrepancy may in part be related to the scale difference between a lab sample and a field measurement, leading to a reduced variability of water retention parameters for the lab data compared to the field data (Diekkrüger, 1990). One element in this is that a measurement on a single (or a few) sample(s) of only about 100-cm^3 cannot adequately represent the spatial variability in soil structure, which is an important factor determining a soil's capacity to retain water. Bork and Driekkrüger (1990) showed how lab- and field-measured water retention curves can differ considerably and the authors concluded that laboratory desorption curves represent the conditions of maximum volumetric water content that may occur in the field at a certain matric potential in the soil. For data use at a regional scale, as often is the case in crop modeling, doing field measurements are no attractive option, so use of lab data or PTFs is almost inevitable. For sandy soils, it was well-known that the commonly used −33 kPa is not optimal, and often a matric potential of −10 kPa is used instead. This could not be confirmed by the data presented here, because of the methods compared, only Method_Baumer–Rice applies to very sandy soils and also allows estimation at −10 and −33 kPa.

According to Ratliff et al. (1983), the lab-measured DUL overestimated for SIL, SICL, SIC, but we found it to occur only with SIL, SICL, SIC and CL. An underestimation occurred according to Ratliff for DUL for S, SL, SCL, but we found it most pronounced for S, CL, SIL, L,

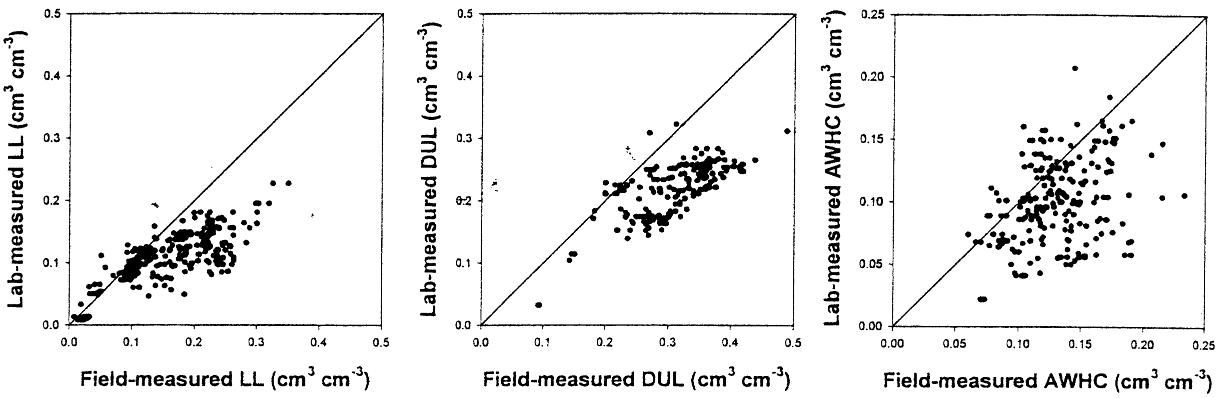

Fig. 6. Lab-measured versus field-measured water retention data. Field capacity (DUL) was measured in the lab at −33 kPa and wilting point (LL) was measured at −1500 kPa; plant-extractable water (AWHC) equals DUL−LL. The data were a subset of the field- and lab-measured data of Ratliff et al. (1983), Ritchie et al. (1987).

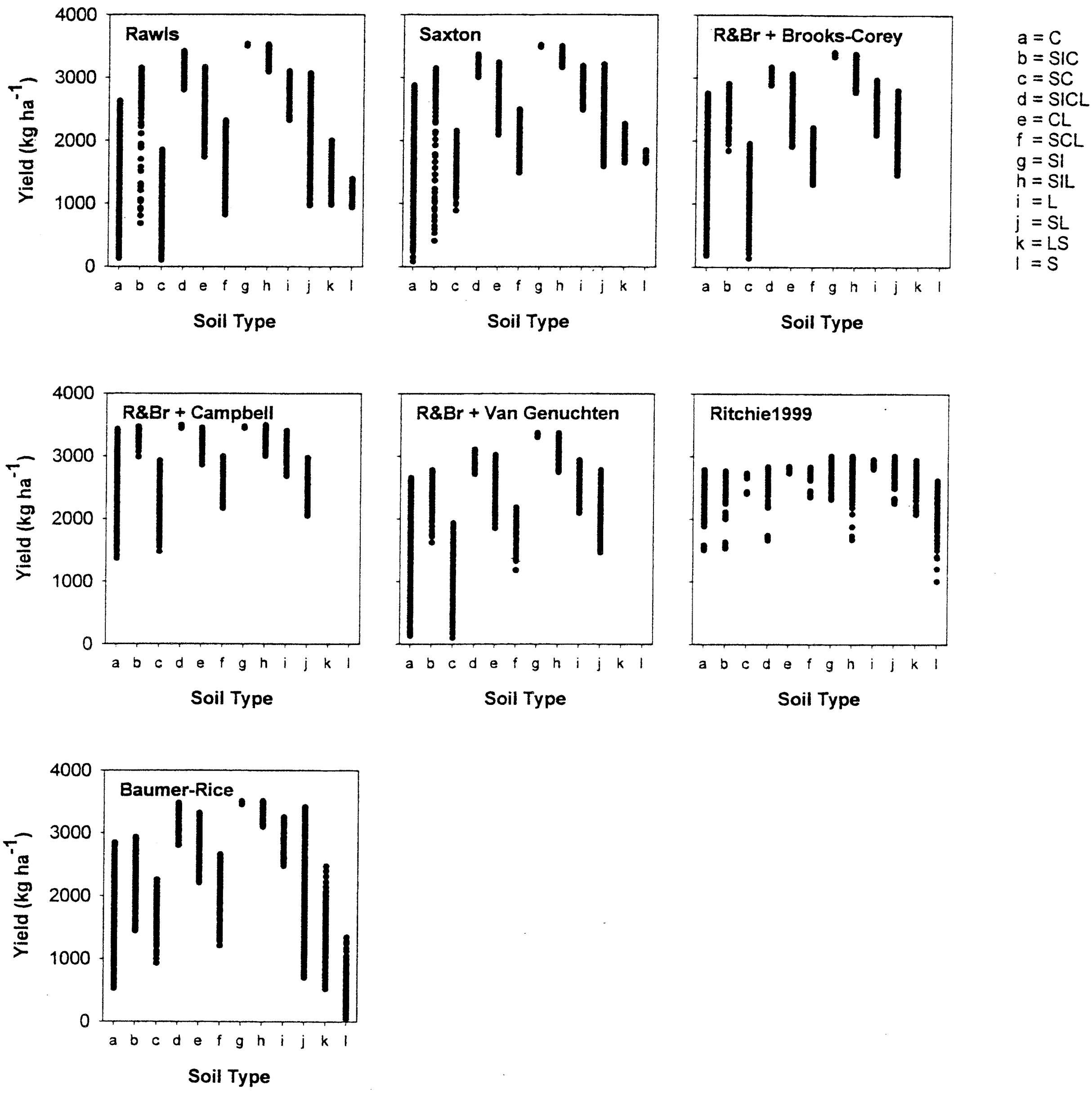

Fig. 7. Simulated soybean yields for > 5000 (imaginary) homogenous soils, each composed of one of the texture combinations that cover the full texture triangle in steps of 1%, arranged by soil type. Seven different water retention-estimation methods were used for parameterizing the DSSAT model. Each dot represents the average of 11 runs with different weather data of Tifton. For the soil types, see Nomenclature in the Introduction.

SCL. As a result of the inaccurate estimation of both LL and DUL, the AWHC is not accurate either: it was overestimated by up to 0.063 $cm^3\,cm^{-3}$ (mostly SI, SIL, SICL) and underestimated by up to 0.132 $cm^3\,cm^{-3}$ (mostly L, SIL, SICL, SIC, SL, CL). These errors in estimat-

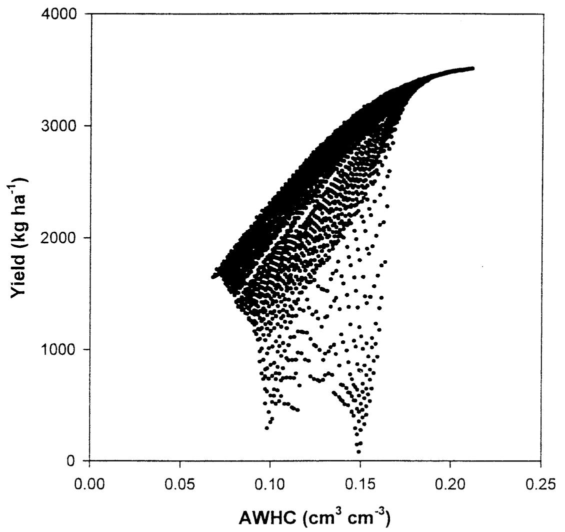

Fig. 8. Same yield data as in Fig. 7, but only with the Method_Saxton and with the yield data organized as a function of the plant-extractable water AWHC.

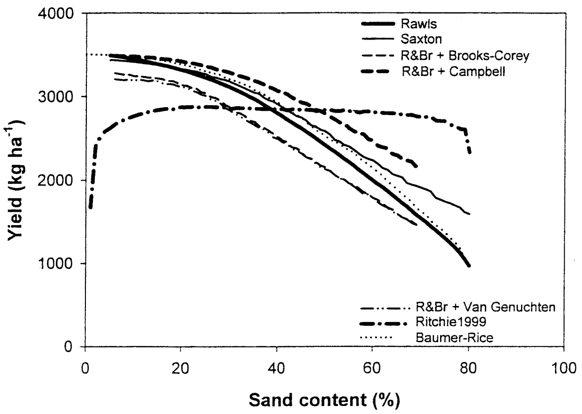

Fig. 9. An extract from the data with the Method_Saxton in Fig. 7 for a limited texture range: clay is set to 20% and sand varies from 0 to 80%.

ing field available-water-holding limits by using lab-measured data would result in major errors in predicting crop growth and yields.

This clearly points to the need for more field-measured data on the critical volumetric water contents, and for better relationships that can be used to interpret lab-measured data in terms of what they mean in the field. The commonly used −33 and −1500 kPa for, respectively, DUL and LL seem to be too inflexible. There has not been agreement on −33 or −10 kPa for DUL of the more sandy soils (Ratliff et al., 1983); only the method of Baumer and Rice (1988) uses a variable matric potential for DUL.

A remaining point of difference between lab- and field-measured water retention data is that under tropical conditions, the temperature inversion in the soil profile between day and night (Day: topsoil = warm, deep soil = cold; Night: topsoil = cold, deep soil = warm) may lead to an upward water transport in the profile at night, especially when the soil gets drier (Philip and De Vries, 1957; Rose, 1968a,b; Amézquita, 1981). Plants often survive in this way under conditions that based on potted-plant experiments in a greenhouse are seen as mortal.

7. Results and discussion on step 3: impact of different estimates for simulated yield

Simulation runs were done with the CROPGRO-Soybean model (Boote et al., 1998) in DSSAT for a soybean crop under 11 years of weather conditions for Tifton. The full array of > 5000 texture combinations were simulated. Fig. 7 shows the average simulated annual yields plotted against the soil type. As each soil type covers many texture combinations, there will not be just one yield estimate, if one only knows the soil type but not the precise soil texture. Instead, there will be a wide range of yield estimates, which may vary from zero to 3000 kg ha^{-1} (e.g. Method_Saxton with a clay soil). It is clear that one needs soil-texture data for crop simulations.

In DSSAT, a high AWHC does not necessarily mean that the crop has easy access to the water, because the water uptake capability of roots is made a function of the LL: a higher LL means a lower water uptake at a certain soil-water content. This results in it that a given AWHC does not mean the same—or even a similar—yield, as e.g., an AWHC of 0.15 cm^3 cm^{-3} gives a higher water uptake (and thus probably a higher yield) if it is with a DUL and LL of, respectively, 0.20 and 0.05

cm^3 cm^{-3}, than with 0.40 and 0.25 cm^3 cm^{-3}. Fig. 8 illustrates this for just one of the water retention methods used (Method_Saxton); these are the same data as used in Fig. 7. This is very confusing characteristic of the DSSAT model, which deserves further attention. The simulated-yield as a function of sand content of the soil is shown in Fig. 9, where the clay content was fixed at 20% and sand content covered the full spectrum from 0 to 80%. Most estimation methods follow a similar pattern in the resulting yield simulations, with the exception of Method_Ritchie1999. With this method, yields do not vary a lot with texture; besides at the two extremes of the curve (i.e. low and high sand content). The strong decline at very low sand contents is due to the high LL that this method estimates for such textures (up to 0.278 cm^3 cm^{-3}), which (as explained above) results in a lower simulated water uptake and thus lower yield. Of all the other methods, only Method_Baumer–Rice applies to such soils, but with LL estimates that are far lower (<0.126 cm^3 cm^{-3}).

8. Conclusions

The wide variation of the soil-water retention estimates among methods and within one soil type stresses some very important points for crop modelers:

(1) One cannot parameterize a crop model by simply basing the water retention parameters on the soil type; precise texture data are needed for each soil layer.

(2) The wide discrepancy between methods is a major source of concern and it is not easy to make recommendations on which method to use for which soil. The Method_Saxton, though, performed best among those compared in this paper, but this does not apply to all soils. For very sandy soils, no method performed well.

(3) Lab-measured water retention data seem to be an acceptable alternative to field-measured data for LL values of less than 0.13 cm^3 cm^{-3}; for higher LL values the lab-measured value is likely to underestimate LL. For DUL, lab-measurements are not a good alternative for field-measurements, besides the uncertainty about which matric potential should be used. Alternative approaches are needed for this, provided that they balance between labor input and data quality. The methodology used by Braga (2000) of doing time series of soil-water measurement and using these in an optimization technique to obtain an estimate of LL and DUL could be an interesting alternative for expensive experiments of the type Ratliff, Ritchie et al. did to obtain field-measured water retention data. This optimization method deserves further attention.

(4) Concerning the specific methods compared here, the following conclusions seem to be appropriate:

- It is recommended not to use Method_Ritchie1987 in its original form. If one has measured BD data, the soil has a low SOM content and one corrects the typo of '197' instead of '17', this method may still be acceptable if used within the range of soil types found in the field-measured data.
- The Method_Rawls and Method_Saxton are very similar. Method_Saxton uses only texture data as input, while Method_Rawls also uses SOM and BD, and gives the option of using (lab?)-measured DUL and LL. For soils with a high SOM content or an uncommon BD, The Method_Rawls is more suitable. The Method_Rawls–Brakensiek varies considerably depending on the follow-up method used (Brooks–Corey, Campbell or Van Genuchten), but one must use porosity instead of saturated water content as input, which may lead one to question its use. Van Genuchten and Brooks–Corey give very similar results; Campbell is the least suitable.
- The Method_Ritchie1999 seems an oversimplification by giving all non-sandy soils the same AWHC. Its DUL estimate seems quite good for intermediate textures, but LL not so (as it depends on AWHC).
- Though the Method_Baumer–Rice covers all soil types, it is not clear whether it is generally applicable or mainly to cracking clays. It estimates very high porosity values.

From a crop modeling point of view, we would like to call on hydrologists to come up with a wider dataset of field-measured data, which could be used to define which matric potential would be appropriate for DUL in what type of soil. The data could also serve to derive an estimation method exclusively based on field-measured data, along the lines of the flawed Method_Ritchie1987.

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