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Environmental Modelling & Software



journal homepage: www.elsevier.com/locate/envsoft

Reanalysis of a global soil database for crop and environmental modeling

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A R T I C L E I N F O

Article history: Received 3 September 2011 Received in revised form 21 February 2012 Accepted 25 February 2012 Available online 24 March 2012

Keywords: WISE 1.1 Soil reanalysis database DSSAT Quality control Global soil database Model applications

ABSTRACT

There is an increased need for detailed soil information that can be used for applications of crop and environmental modeling. The goal of this project was to conduct a reanalysis of the ISRIC-WISE 1.1 Soil Profile Dataset. As part of the procedures, the soil reanalysis database was fitted to the standard formats of the International Consortium for Agricultural Systems Application (ICASA). Thus, the soil reanalysis database tailors dynamic crop models such as the Cropping System Model (CSM) of the Decision Support System for Agrotechnology Transfer (DSSAT). During the reanalysis, the physical and chemical parameters of the soil profiles were revised and estimated, where necessary and possible, using pre-established ranges given by the literature and correlations among other more stable variable. To evaluate each of the 3404 reanalyzed soil profiles, the CSM-CERES-Maize model was run for a standard crop management scenario using both the original and the new improved soil databases. Nine hundred seventy-eight soil profiles were considered to be not useful during the reanalysis due to missing values for one or more critical variables and were, therefore, not considered for quality control procedures. A pre-diagnostic for only nitrogen and soil organic carbon in the original dataset showed 70% and 5% of missing values respectively. A sensitivity analysis based on crop simulations comparing the original and the reanalyzed soil databases, showed that 1294 soil profiles yielded different results due to improvement of either the original data or improved conversion procedures. The details and considerations for detecting missing and erroneous values and for estimating soil variable values are presented in this paper for further use. The final soil reanalysis global database contains 3404 soil profiles and is available at https:// harvestchoice.wufoo.com/forms/download-wisol.

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1. Introduction

Computer simulation models have recently become more common and acceptable for impact assessment studies and for supporting policy decisions on different temporal and spatial scales. Soil data are in high demand as inputs for running simple to complex models including soil erosion models (i.e., Flanagan and Nearing, 1995; Williams et al., 1983), hydrologic models (i.e. Neitsch et al., 1999), crop simulation models (i.e., Tsuji et al., 1998; Hoogenboom, 2000; Baigorria et al., 2007; Boote et al., 2010) and other type of models (Wu and Liu, 2012; Panagos et al., 2012; Lippe et al., 2011; Baigorria and Romero, 2007). To apply these models, detailed, extensive, quantitative and geo-referenced databases covering small to large regional areas are needed. Unfortunately, often these databases are neither in the formats nor in the specific dimensions required for crop and environmental models (Batjes, 2009).

The International Soil Reference and Information Centre (ISRIC) developed a detailed geo-referenced soil database, entitled 'World Inventory of Soil Emission Potentials' (WISE), including Version 1.0 (Batjes, 1995) and Version 1.1 (Batjes, 2002). After this study was concluded, a new version named "ISRIC-WISE Harmonized Global Soil Profile Dataset" (WISE 3.1) was released that holds selected attribute data for 10 253 soil profiles (Batjes, 2008, 2009). Gijsman et al. (2007) used WISE 1.0, containing 1125 profiles, of which 836 were converted into a format suitable for the crop simulation models within DSSAT (Jones, 1998; Hoogenboom et al., 2004). The remaining soil profile descriptions had missing values or contained suspect values. WISE 1.1 was used to demonstrate the important role that large soil databases can play in the understanding and

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^{1364-8152/\$ –} see front matter \odot 2012 Elsevier Ltd. All rights reserved. doi:10.1016/j.envsoft.2012.02.018

modeling of the global distribution of soils and their properties (Gray et al., 2009, 2011). However, it is important to realize that correcting and estimating missing values for these databases potentially increases the number of valid soil profiles to allow working in more areas and at higher resolution with simulation models.

A reanalysis of the ISRIC-WISE 1.1 Soil Profile Dataset will produce a new soil reanalysis global database for crop modelers based on the standard format developed by the International Benchmark Sites Network for Agrotechnology Transfer (IBSNAT; Uehara and Tsuji, 1998; Hunt et al., 2001). This ready-to-use database will allow scientists to focus on science rather than on reformatting data and estimating missing values and inconsistencies in the data by themselves, thus supporting global efforts as the Agricultural Model Intercomparison and Improvement Project (AgMIP; http://www.agmip.org).

This paper addresses two main questions. First, is it possible to detect discrepancies in physical and chemical soil properties by analyzing relationships with other soil properties in the same and/ or adjacent soil horizons? Second, after detecting these differences, is it possible to either correct or estimate these values based on established theoretical ranges, relationships and empirical algorithms? The main objectives of the present work were (i) to create a quality control method to detect and correct/estimate suspected values and to fill in missing values of physical and chemical soil properties found in the ISRIC-WISE 1.1 Soil Profile Dataset, (ii) to create a new soil profile database for agricultural and environmental modeling purposes only, and (iii) To compare the performance of the soil profiles before and after the reanalysis process by running virtual experiments using the CSM-CERES-Maize model (Jones and Kiniry, 1986; Jones et al., 2003).

This soil database includes soils that are and are not considered for agricultural purposes. However, due to the lack of other sources of soil data, especially for modeling purposes in several parts of the world, most of the described soil profiles were assumed to be agricultural soils that could be used for either food, feed, fiber, or fuel production.

2. Database description

During the 1990s, the WISE soil database was developed by the International Soil Reference and Information Centre (Batjes and Bridges, 1994). WISE version 1.0 included 1125 soil profiles from around the world (Batjes, 1995). In 2002, WISE Version 1.1 was released to expand the availability of detailed soil profiles (Batjes, 2002). This homogenized data contains 4382 soil profiles from 123 countries across the world. Each soil profile is geo-referenced and classified using both the original Legend (1974) and the Revised Legend (1988) of the Food and Agriculture Organization (FAO) – United Nations Educational, Scientific, and Cultural Organization (IUSS Working Group WRB, 2006; Batjes, 2002). This WISE soil data encompasses soil profiles released by FAO, ISRIC, and USDA-NRCS, and profiles collated at ISRIC from national soil survey reports and other publications. The soil descriptions from USDA-NRCS follow the methodology of the Soil Survey Manual (USDA-SCS-Soil Survey Staff, 1983). However, the chemical and physical analyses for the corresponding soil samples were conducted in different laboratories, using the common methodologies that were in use in the countries from which the profiles were obtained. Therefore, a comparison between data held by FAO with those analyzed at NRCS and ISRIC might not always be necessarily possible (Vogel, 1994; Batjes, 2002).

Table 1 shows the number of soil groups according to FAO summarized by continent. Soil profile information consisted of (i) general data such as location, soil class, color, and depth, (ii)

Soil class	Africa	Asia	North America	Central & South America	Europe	Oceania
Acrisol	117	32	8	46	2	7
Alisol	5	33	5	14	5	_
Andosol	12	25	1	51	15	5
Anthrosol	_	20	1	_	3	_
Arenosol	187	12	4	10	5	1
Calcisol	35	59	9	3	12	_
Cambisol	100	189	20	57	113	15
Chernozem	9	11	10	_	18	_
Ferralsol	129	40	1	63	2	11
Fluvisol	64	181	6	23	44	4
Glevsol	80	40	7	19	37	2
Grevzem	_	1	4	_	1	_
Gypsisol	1	9	2	1	1	_
Histosol	_	_	_	2	2	_
Kastanozem	_	4	9	7	7	1
Leptosol	21	15	1	13	13	1
Lixisol	49	11	1	14	_	-
Luvisol	189	51	26	21	89	10
Nitisol	8	14	4	24	_	2
Phaeozem	37	15	19	71	29	1
Planosol	18	1	4	14	7	2
Plinthosol	6	7	-	5	1	-
Podzol	10	6	1	5	24	3
Podzoluvisol	_	1	2	-	7	-
Regosol	33	11	1	16	6	1
Solonchack	20	26	3	6	6	_
Solonetz	19	17	5	12	2	3
Vertisol	121	64	4	25	27	9
Xerosol	2	_	_	_	_	_
Yermosol	_	_	-	-	-	1
TOTAL	1272	895	158	522	478	79

The soil groups, according to FAO (1990) and included in WISE v. 1.1^a.

^a Soil groups were summarized by continent. The value indicates the number of soil profiles in WISE 1.1 database.

physical properties such as hydraulic coefficients, bulk density, and soil texture, and (iii) chemical properties such as soil organic carbon, nitrogen concentration, and pH, among others.

3. Methods

Possible discrepancies in the database were identified through (i) the comparison of each physical and chemical property within the range of values established through a detailed literature search, (ii) the gradient between adjacent soil layers, and (iii) the relationships between parameters in the same soil layer (Kaiser et al., 2007: Post et al., 2001; Wu et al., 1999; Ross and Bartlett, 1996; Aitken, 1992; Saxton et al., 1985; Pionke and Corey, 1967; Tucker, 1954). If any discrepancies were found, the data were corrected based on established ranges or correlations with other soil properties, such as percentage of nitrogen as a function of organic carbon content. For missing values, we focused on two critical soil parameters, soil organic carbon and soil nitrogen. Chemical parameters, such as iron, manganese and sulfur concentrations, as well as soil phosphorus isotherms A and B, were not considered in this analysis. The technical process involved an automatic computer routine to detect soil profiles showing discrepancies and/or missing values. Missing values were automatically calculated using algorithms based on the rules described in Table 3; however, after being identified, discrepancies were manually evaluated, otherwise special soils with extreme values for some parameters would not be modified.

3.1. Identification of discrepancies and methods used for correction

Rules were applied to most soil parameters (Table 2) to verify if the value under evaluation fell within a range of values already established in the literature. For particular soil types with a high organic matter content, e.g. Histosols, Andosols, Chernozems and Kastanozems (both equivalent to Mollisols in the Soil Taxonomy nomenclature), or high in vermiculite clay (e.g. Vertisols), there are some unique properties resulting from these characteristics which values might exceed from those of mineral soils (e.g. organic carbon content, cation exchange capacity). These values are reasonable for these particular soils. Table 3 shows the rules that were applied if any inconsistencies were identified for most soil parameters. Tables 4and 5 shows the rules for drainage rate, and runoff curve number. A brief description of what was done when a discrepancy was identified is described next. The established limits for maximum and minimum values and associated references are shown in Table 3.

Soil data requirements for a daily time-step crop simulation model, such as the Cropping System Model (CSM) (after Gijsman et al., 2007).

Parameter name	Meaning	Units
General data		
SLTX	Texture code of surface layer	unitless
SLDP	Soil depth	cm
SLDESCRIP	Soil description or local classification	unitless
COUNTRY	Country	unitless
LAT	Latitude	unitless
LONG	Longitude	unitless
SCSC FAMILY	Soil class	unitless
General and soil si	urface information	
SCOM	Soil color (Munsell color system)	unitless
SALB	Albedo	unitless
SLU1	Evaporation limit	cm
SLDR	Drainage rate	fraction day ⁻¹
SLRO	Runoff curve number	unitless
SLNF	Mineralization factor	0–1 scale
SLPF	Soil fertility factor	0–1 scale
SMHB	pH in buffer determination method	unitless
SMPX	Extractable phosphorus determination code	unitless
SMKE	Potassium determination method	unitless
First tier	Death antilless of large	
SLB	Depth until base of layer	cm
SLIMH	Master norizon	$m^3 cm^{-3}$
SLLL	Drained upper limit	$cm^3 cm^{-3}$
SDUL	Saturated upper limit	$cm^3 cm^{-3}$
SPCE	Saturated upper minit	
SKGP	Saturated hydraulic conductivity	o=1 scale
SEDM	Bulk density (moist)	σcm^{-3}
SLOC	Soil organic carbon concentration	% CIII
SLOC	Clay (< 0.002 mm)	%
SUSI	Silt $(0.002 - 0.05 \text{ mm})$	%
SLCF	Coarse fraction (>2 mm)	%
SUNI	Total nitrogen concentration	%
SLHW	pH in water	unitless
SLHB	pH in buffer	unitless
SCEC	Soil cation exchange capacity	$\text{cmol}^{(+)} \text{kg}^{-1}$
SADC	Soil adsorption coefficient	0–1 scale
	(anion exchange cap.)	
Second tier		
SLPX	Extractable soil phosphorus concentration	$mg kg^{-1}$
SLPT	Total soil phosphorus as P concentration	mg kg $^{-1}$
SLPO	Soil organic phosphorus concentration	${ m mg}~{ m kg}^{-1}$
CACO ₃	Soil CaCO ₃ concentration	%
SLAL	Soil aluminum concentration	mg kg ⁻¹
SLFE	Soil iron concentration	mg kg ⁻¹
SLMN	Soil manganese concentration	mg kg ⁻¹
SLBS	Soil base saturation	%
SLPA	Soil phosphorus isotherm A	mmol kg ⁻¹
SLPB	Soil phosphorus isotherm B	mmol kg ⁻¹
SLKE	Exchangeable potassium soil concentration	$cmol^{(+)} kg^{-1}$
SLMG	Exchangeable magnesium concentration	$cmol^{(+)} kg^{-1}$
SLNA	Exchangeable sodium concentration	$cmol^{(+)} kg^{-1}$
SLSU	Soil sulfur concentration	$cmol^{(+)} kg^{-1}$
SLEC	Soil electric conductivity	$dS m^{-1}$
SLCA	Soil calcium concentration	cmol ⁽⁺⁾ kg ⁻¹

a. Soil organic carbon (SLOC): Soil organic carbon content seems to accumulate in the topsoil and tends to decrease with depth. A high organic carbon value between layers showing low values could be related to a buried horizon. This was verified with the corresponding master soil horizon. If no identification of a master soil horizon was shown, the values were left as is. If the soil horizon was correctly described, the values were left as is too. A buried horizon should show a 'b' suffix after the buried A, E, or B horizon designators. If the buried horizon was identified, then the values were left as is too. High values of organic carbon in mineral soils that exceeded the maximum limit of 5% were set to this limit, except for Andosols, Chernozems, Kastanozems, and Histosols.

b. Total nitrogen concentration (SLNI): The rules that were applied to soil organic carbon were also applied to total nitrogen concentration. The values of total nitrogen in mineral soils that exceeded the maximum of 0.5% were set to this limit, except for Andosols, Chernozems, Kastanozems, and Histosols.

c. Calcium carbonate content (CaCO₃): Any value that exceeded 50% was set to this maximum limit, except for calcareous soils.

d. Cation exchange capacity (SCEC): The upper limit for most mineral soils was considered 45 $cmol^{(+)}$ kg⁻¹. The values that exceeded this upper limit were set to this value, except for Vertisols which were left as is. Higher values were permitted for Histosols.

e. Soil bulk density (SBDM): Normal values for SBDM range between 0.5 and 1.8 g cm⁻³ for soils with agricultural purposes. Any value that exceeded the upper limit was set to 1.8. Values below the minimum limit were taken to 0.5, except for Histosols, which bulk density could reach 0.2 g cm⁻³.

f. Soil pH in water (SLHW) and soil pH in buffer (SLHB): pH in water is the most common method use in the field due to availability of water. pH measured in buffer can use two solutions: Potassium Chloride (KCl, 1 N) or Calcium Chloride (CaCl₂, 0.01 M). The use of KCl is designed to test for the presence of exchangeable aluminum. As a result, the solution pH is lowered. CaCl₂ pH is the standard used in Soil Taxonomy to differentiate acid and nonacid family reaction classes in mineral soils and *euic* and *dysic* family classes in organic soils. The result is a pH measurement that remains somewhat invariable to the seasonal changes in pH (Thomas, 2009), and it is slightly lower than pH measured in water (Conyers and Davey, 1988). Soil pH values should range from 3.5 to 9.0. Any values out of this range were set to either the minimum if the values were below the range or to the maximum limit if the values were above the range, except for sodic soils.

g. Soil saturated hydraulic conductivity (SSKS): Values should range from 0.05 cm h^{-1} for clayey soils to 63 cm h^{-1} for sandy soils. If a value was not suitable for a specific soil texture, a pedotransfer function was used to estimate a new value (Table 3).

h. Exchangeable Calcium (SLCA), Magnesium (SLMG), Potassium (SLKE) and Sodium (SLNA): Values exceeding the limits shown in Table 3 were set to the maximum value, except for saline, sodic, and calcareous soils, as well as in Vertisols.

i. Soil electrical conductivity (SLEC): A limit of 16 dS m⁻¹ was established for soil with agricultural purposes. Any values exceeding this limit were set to the maximum value, except for both saline and saline-sodic soils.

j. Soil aluminum concentration (SLAL): Value should range from 0 in alkaline soils to 12.4 cmol⁽⁺⁾ kg⁻¹ in acid soils. Values above this limit were set to 12.4 cmol⁽⁺⁾ kg⁻¹, except for Acrisols and Ferralsols, which can have values that are higher. At a pH 5.5 and above, exchangeable Al³⁺ is no longer present. Monomeric Al³⁺ is dominant when the soil pH is less than 5.5. Al³⁺ chemistry above a pH of 5.5 is dominated by a complex mixture of hydroxyl-Al ions, many of them highly polymerized and virtually non-exchangeable. Ideally, therefore, there should not be exchangeable aluminum over a pH of 5.5.

k. Hydraulic coefficients: The values for the lower limit of plant extractable soil water (LL) should be less than the values for the drained upper limit (DUL), while values for the DUL should be less than values for the saturated soil water content (SAT).

I. Soil base saturation (SLBS): The soil base saturation ranges from 0 to 100%. It should equal 100% when no $Al^{3+} + H^+$ are available.

m. Minor inconsistencies: When an obvious inconsistency was observed in the database, like misspellings in some words, they were corrected.

n. No corrections: The following parameters were not corrected or estimated because there were no corresponding measurements in the soil profiles: soil sulfur concentration (SLSU), extractable soil phosphorus concentration (SLYX), total soil phosphorus as P concentration (SLPTL), soil organic phosphorus concentration (SLPO), soil iron and manganese concentration (SLFE and SLMN), soil phosphorus isotherms A and B (SLPA and SLPB), and soil adsorption coefficient.

3.2. Procedure followed to estimate missing values

Missing values were represented as -99.0 in the soil profile description, meaning that no data value was measured or stored for a soil parameter. Proper handling of missing values is important for all analyses because values can distort the soil analysis results. The C:N ratio in the organic matter of cultivated surface horizons has an average near 12:1 (Brady and Weil, 1999). Batjes (1996) found that C:N ratios tend to decrease with soil depth. For practical purposes, a C:N ratio equal to 10 was used to estimate either parameter in soil layers with missing values. If both C and N were not available in a soil profile, no estimation was performed.

Estimation of hydraulic coefficients, like SLLL, SDUL and SAT, were estimated according to Saxton et al. (1985). Any other possible estimation was performed accordingly to the proposed rules (Table 3).

3.3. Sensitivity analysis

A sensibility analysis was performed to compare simulations outputs before and after the reanalysis of the soil profiles, while keeping the rest of the model inputs constant. The CSM-CERES-Maize model (Jones et al., 2003; Jones and Kiniry, 1986) was used for this comparison. The virtual experiments were based on a crop management scenario for maize for Gainesville, Florida using well-watered and well-fertilized conditions (Jones et al., 1986, 2003; Hoogenboom et al., 2004). This experiment is one of the standard experimental datasets distributed with DSSAT (Boote et al., 2010). The cultivar used was McCurdy 84aa. Three applications of N fertilizer were applied totalizing 116 kg ha⁻¹. A total of 264 mm of irrigation in 16 applications was applied.

Rules to identify potential discrepancies observed in the WISE soil database.

Soil variable	Range	Reference
Soil color	DSSAT uses brown, red, black, gray, yellow, and yellow-red. Soils that did not have a color code were classified as 'brown'.	Tsuji et al. (1994); Gijsman et al. (2007).
Soil albedo	Albedo is estimated from the soil color or the top layer. Ranges from 0.09 for a black soil to 0.17 for a yellow soil.	Ritchie et al. (1990); Gijsman et al. (2007).
Evaporation limit	Less or equal to 12.0 mm d^{-1} .	FAO (1990).
Clay fraction	0-100%	Gee and Bauder (1986).
Silt fraction	0-100%	Gee and Bauder (1986).
Coarse fraction	0-100%	FAO (2006).
Drainage rate	Seven permeability classes: very poorly drained 0.01), poorly drained (0.05), somewhat poorly drained (0.25), moderately well drained (0.40), well drained (0.60), somewhat excessively drained (0.75), and excessively drained (0.85).	Ritchie et al. (1990).
Runoff curve number	Soils are classified by slope and by hydrologic group, runoff curve number ranges from 61 to 94.	Ritchie et al. (1990).
Mineralization factor	1	Giisman et al. (2007).
Soil fertility factor	1	Gijsman et al. (2007).
Soil depth until the base of the layer	Use only the lower limit of a soil layer or horizon.	Gijsman et al. (2007).
Hyd. coefficients: Lower limit, drained upper limit, and saturated limit.	Values for lower limit should be less than values for drained upper limit. Values for drained upper limit should be less than values for saturated limit. For missing	Saxton et al. (1985).
Bulk density	Values pediotransier equations were used for estimation. $0.5-1.8 \text{ g cm}^{-3}$ for most soils except Histosols that can show low values as 0.2 g cm^{-3} .	Brady and Weil (1999); Wild (1993); FAO (2006)
Soil organic carbon	Most soil surface layers (0.2 m) seldom contain more than 5% soil carbon. High values could be associated with Histosols, Andosols, Czernozems and Kastanozems. It can be estimated from C:N = 10.	Buringh (1984); Batjes (1996); Eswaran et al. (1993); Brady (1990).
Total nitrogen concentration	Values should range between 0 and 0.5%. Higher values could be associated to Histosols, Andosols, Czernozems and Kastanozems, and Histosols. If not data is available, can be estimated from a $C:N = 10$.	Batjes (1996); Brady and Weil (1999).
pH in water(SLHW)/pH in buffer(SLHB)	pH measured in water (SLHW) should range between 3.5 and 9.0. pH measured in buffer (SLHB) should have a value lower than SLHW.	Brady and Weil (1999); Wild (1993); USDA-NRCS (2011).
Soil cation exchange capacity	Range from 0 to 45 cmol ⁽⁺⁾ kg ⁻¹ for most mineral soils. Histosols and Vertisols are the exception, reaching around 150 cmol ⁽⁺⁾ kg ⁻¹ .	Holmgren et al. (1993); Hemni (1980).
Soil CaCO ₃ concentration	<50% for agricultural soils.	Brady and Weil (1999).
Soil aluminum concentration	Range from 0 to 12.4 cmol ⁽⁺⁾ kg ⁻¹ . At pH 5.5 and above exchangeable Al ³⁺ is no longer present. Al chemistry is dominated by a complex mixture of hydroxyl-Al ions, many of them highly polymerized and virtually non-exchangeable	Kamprath (1980); Singh and Talibudeen (1969); Aitken (1992); Dong et al. (1999); Hsu and Rich (1960); Marion et al. (1976); Lathwell and Peech (1964)
Soil base saturation	Range from 0 to 100%. Equal to 100% when no $Al^{3+} + H^+$ is available in soil solution.	Brady and Weil (1999).
Exchangeable cations	Ca: $<35 \text{ cmol}^{(+)} \text{ kg}^{-1*}$ Mg: $<20 \text{ cmol}^{(+)} \text{ kg}^{-1*}$ K: $<30 \text{ cmol}^{(+)} \text{ kg}^{-1}$ Na: $<20 \text{ cmol}^{(+)} \text{ kg}^{-1}$ *Most Ca ²⁺ and Mg ²⁺ values on Vertisols were not modified since they exceeded greatly the established limits.	Hendershot and Duquette (1985); Tucker (1954).
Soil electrical conductivity	<16 dS m ⁻¹ for agricultural soils (except very saline soils).	Brady and Weil (1999).
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Table 4

Rules to identify potential discrepancies observed in drainage classes in the WISE database matched with the permeability classes of DSSAT in agreement with Ritchie et al. (1990), and runoff curve numbers (Ritchie et al., 1990) (after Gijsman et al., 2007).

Soil depth (cm)	Clay + Silt (%)	Drainage rate (mm h^{-1})	Hydrological Group	Runoff curve number (at different slope angles)			
				0-2%	2-5%	5-10%	>10
≥150	≤15	0.75–0.85	A	61	64	68	71
80-150	≤15	0.60-0.75	В	73	76	80	83
70-80	>15	0.40-0.60	С	81	84	88	91
60-70	>15	0.25-0.40	С	81	84	88	91
	Clay						
60-80	>50	0.05	D	84	87	91	94
<50	>50	0.01	D	84	87	91	94

Source: Ritchie et al. (1990).

Rules to identify potential discrepancies observed in saturated hydraulic conductivity in the WISE 1.1 database.

Table 6

Number of soil profiles with at least one discrepancy in the WISE 1.1 database, and number/percentage of soil profiles corrected.

Soil texture	Hydraulic conductivity (cm h^{-1})		
Sand	63.4		
Loamy sand	56.2		
Sandy loam	12.3		
Silt loam	2.59		
Loam	2.52		
Sandy clay loam	2.27		
Silty clay loam	0.61		
Clay loam	0.90		
Silty clay	0.36		
Clay	0.47		

Source: Clapp and Hornberger (1978).

4. Results and discussion

4.1. Error correction procedure

Of the 4382 soil profiles in the original ISRIC-WISE v 1.1 soil database there were 249 profiles with discrepancies and 1696 profiles with missing values. Many of these were corrected but 978 could not be, meaning there were ultimately 3404 valid and usable profiles in the corrected database (Fig. 1). Tables 6 and 7 show the number and the percentage of discrepancies that were corrected based on soil profiles and soil layers, respectively.

a. Organic carbon in the soil (SLOC): Ninety-two soil profiles showed discrepancies for organic carbon values (Table 6). Just four of these profiles were corrected. The rest showed very high organic carbon values which values were accepted since these soil profiles were classified as organic soils (Andosols, Molisols or Histosols). From the four soil profiles corrected, one showed a soil layer with a high concentration of organic matter at the bottom of the soil profile. As it was not a buried horizon (Table 7), the value was replaced by the value of the overlying soil layer.

b. Total nitrogen concentration (SLNI): One hundred and fiftyfour soil profiles showed discrepancies for this parameter because their values were higher than normal. These potential errors were double checked, and the soil profiles confirmed to be classified as

Soil parameters	# of soil profiles showing at least one discrepancy	# of soil profiles which discrepancies were corrected	% of soil profiles with discrepancies corrected
SCOM	3	3	100
SALB	3	3	100
SLU1	0	0	0
SLDR	0	0	0
SLRO	0	0	0
SLNF	0	0	0
SLPF	0	0	0
SLB	1	1	100
SLLL	2	2	100
SDUL	5	5	100
SSAT	6	6	100
SRGF	0	0	0
SSKS	58	12	21
SBDM	17	1	6
SLOC	92	4	4
SLCL	0	0	0
SLSI	0	0	0
SLCF	0	0	0
SLNI	154	0	0
SLHW	208	81	39
SLHB	84	71	85
SCEC	957	19	2
CACO ₃	76	2	3
SLAL	142	0	0
SLBS	5	5	100
SLKE	636	0	0
SLMG	681	3	0
SLNA	668	14	2
SLEC	86	6	7
SLCA	740	11	1
TOTAL	4624	249	5.4

Andosols, Molisols and Histosols. Therefore, these data were not corrected (Table 6).

c. Calcium carbonate content (CaCO₃): There were 76 soil profiles showing discrepancies for CaCO₃ values. These values generally exceeded the theoretical limit of 50% and were normally



Fig. 1. World map showing the location of all soil profiles in the reanalyzed global soil database for crop and environmental modeling.

Number of soil layers with at least one discrepancy in the original WISE 1.1 database, and number/percentage of soil layers corrected.

Soil	# of soil layers	# of soil layers which discrepancies	% of soil layers with discrepancies
purumeters	one discrepancy	were corrected	corrected
SLB	1	1	100
SLLL	2	2	100
SDUL	5	5	100
SSAT	12	12	100
SRGF	0	0	0
SSKS	83	16	19
SBDM	24	1	4
SLOC	129	4	2
SLCL	0	0	0
SLSI	0	0	0
SLCF	0	0	0
SLNI	212	0	0
SLHW	452	192	42
SLHB	187	159	85
SCEC	3460	6	0
CACO ₃	152	2	1
SLAL	303	0	0
SLBS	7	7	100
SLKE	1975	0	0
SLMG	2293	0	0
SLNA	2163	21	1
SLEC	281	10	4
SLCA	3325	6	0
TOTAL	15 066	444	2.9

found at a depth of 20–50 cm below the soil surface. Carbonates in soils are either residues of the parent material or the result of neo-formation of secondary carbonates (FAO, 2006). Only two soil profiles were corrected (Table 6) which did not correspond to a calcaric soil. These 2 profiles represented 2 soil layers (Table 7).

d. Cation exchange capacity (SCEC): From the total database, 957 soil profiles showed inconsistencies in CEC values. They were observed mostly in Vertisols. These soils have a high content of a type of clay called vermiculite, which is high in negative charges, leading to high values of CEC. These apparent inconsistencies also observed in soils with a high amount of organic carbon content, like Molisols or Andosols, showing values higher than 45 cmol⁽⁺⁾ kg⁻¹. These values were accepted. Only 19 soil profiles needed corrections because the values were extremely high. The values were modified to the maximum suggested range.

e. Soil bulk density (SBDM): Some volcanic soils showed bulk density values that were less than 0.5 g cm^{-1} , but never lower than 0.2 g cm⁻¹, due to the high amount of organic carbon in the soil (>10%). Only one profile (one soil layer) was corrected (Tables 6 and 7).

f. Soil pH in water (SLHW) and in soil pH in buffer (SLHB): Two hundred and eight soil profiles (equivalent to 452 soil layers) showed discrepancies in pH values (SLHW). The most common discrepancy was finding pH values that were higher than 5.5 and exchangeable aluminum was available. No correction was done (Tables 6 and 7). Eighty-one soil profiles showed values for pH determined in buffer that were higher than pH determined in water. For these few cases were both results were reported, pH values determined in buffer were set equal to the values obtained using water. These profiles corresponded to 159 soil layers and all of them were corrected.

g. Soil saturated hydraulic conductivity (SSKS): There were 58 soil profiles that showed some inconsistencies in the data. Just 12 of them were corrected since their values did not correspond to the soil texture category (Table 6). The corrected soil profiles were equivalent to 16 soil layers (Table 7).

h. Exchangeable Calcium (SLCA), Magnesium (SLMG), Potassium (SLKE) and Sodium (SLNA): The values for exchangeable calcium and magnesium for the Vertisols exceeded the established limits but were left as is. Only 11 soil profiles were corrected for calcium, and 3 for magnesium, where the values were modified to the maximum accepted value. Less than 1% of the soil profiles had erroneous values for these parameters. Sodic soils normally showed higher amounts of exchangeable sodium than other soil types. Only 2% of these soils were corrected. The pH values for these soils were 8.5 or higher (Tables 6 and 7).

i. Soil electrical conductivity (SLEC): Six out of 86 soil profiles had potential discrepancies for soil electrical conductivity and were corrected. The rest were left as is since most of them corresponded to saline soils, which normally have very high electrical conductivity values (higher than 16 dS m^{-1}).

j. Soil aluminum concentration (SLAL): There were some few cases where soil aluminum concentration exceeded the established limit of 12.4 cmol⁽⁺⁾ kg⁻¹. However, these soils corresponded to the soil groups of Ferralsols and Acrisols, very acid soils, and the values were not corrected. There were 142 soil profiles, equivalent to 303 soil layers, showing exchangeable Al^{3+} when soil pH was slightly higher than 5.5 (around 5.6–5.7). These values were not modified, since these values repeated consistently, and because it is possible to find soluble Al^{3+} under these pH values (Pionke and Corey, 1967).

k. Hydraulic coefficients: There were two, five and six soil profiles with errors in the SLLL, SDUL and SSAT parameters, respectively. New values were estimated for these soil parameters for all soil profiles according to Saxton et al. (1985).

I. Soil base saturation (SLBS): There were 5 alkaline soil profiles that had values for the soil base saturation that were not equal to 100%, although the sum of cations was equal to their respective CEC. These values for SLBS were therefore changed to 100%.

m. Minor inconsistencies: There were three soil profiles were found with errors in soil color, three soil profiles with errors in albedo, and one soil profile with an error in soil depth. The soil color errors turned out to be misspellings, and these were corrected. Albedo was corrected based on the soil color. Soil depth in one layer was estimated based on the sequence of the adjacent soil layers.

4.2. Results on estimating missing values

Tables 8and 9 show the numbers of soil profiles and soil layers with missing values. These numbers are also expressed in percentage, based on the total number of soil profiles or soil layers. The estimation of missing values was focused on soil carbon and nitrogen, as well as on physical properties such as SLLL, SDUL and SSAT.

Overall, 2361 soil profiles showed missing values for nitrogen. The recovered soil nitrogen values reached 1647, representing 70% of the soil profiles with missing soil nitrogen values (Table 8). Based on soil layers, there were a total of 8310 soil layers with missing soil nitrogen values. From these, 6831 soil layers with nitrogen missing

Table 8

Number of soil profiles with at least one missing value in the WISE 1.1 database, and number/percentage of soil profiles corrected.

Soil parameters	# of soil profiles showing at least one missing value	# of soil profiles which were corrected	% of soil profiles corrected
SLLL	5	5	100
SDUL	5	5	100
SSAT	5	5	100
SLOC	748	34	5
SLNI	2361	1647	70
TOTAL	3124	1696	54.3

 Table 9

 Number of soil layers with at least one missing value in the WISE 1.1 database, and number/percentage of soil layers corrected.

Soil parameters	# of soil layers showing at least one missing value	# of soil layers which were corrected	% of soil layers corrected
SLLL	5	5	100
SDUL	5	5	100
SSAT	5	5	100
SLOC	1525	46	3
SLNI	8310	6831	82
TOTAL	9850	6892	70.0

values were estimated, representing 82% of soil nitrogen data (Table 9). Only 5% of the soil profiles with missing values were recovered using the C:N ratio to estimate soil organic carbon, which represented 34 out of 748 soil profiles with missing soil organic carbon data (Table 8). These soil profiles were equivalent to 46 soil layers (Table 9). Only five soil profile descriptions showed missing values in the hydraulic coefficient parameters (SLLL, SDUL, and SSAT). They all were estimated using pedotransfer functions (Saxton et al., 1985).

4.3. Sensitivity analysis

The performance of the CSM-CERES-Maize model was analyzed using the 3404 valid soil profiles from the original ISRIC-WISE v 1.1 soil database, and the reanalyzed soil profiles. The simulations with the CSM-CERES-Maize model were conducted successfully with all the corrected soil profiles. When using the original valid soil profiles the CSM-CERES-Maize model did not operate with 9 soil profiles, and resulting with values of -99 in the output files. After correcting these profiles, the CSM-CERES-Maize model worked with these 9 soil profiles. Problems were observed for the soil depth parameter (e.g., the third layer was deeper than the fourth layer) and in the nomenclature of the soil layers. There were two soil profiles that resulted in a zero yield, both before and after the correction (WI_LPJO029 and WI_LPUY049). These two soils were classified as Leptosols and both had only one soil layer with a maximum depth of 5 cm.

When comparing the simulated crop yield outputs using the reanalyzed versus the original valid soil profiles, there were 1294 simulated results that were different, representing 38% of the WISE v 1.1 database. Further analysis showed that differences in crop yield ranged from -4.8% to 3.5% when soil profiles were aggregated according to soil groups. For example, Nitosols, Podzols, Regosols, Solonchaks, Solonetz, and Acrisols showed increments in simulated yields in the order of 3.4, 1.2, 3.5, 1.5, and 0.26%, respectively. Soils in this group were characterized by their low fertility, or by having salt accumulation or sodium problems. On the other hand, simulated crop yields decreased in Gypsisols, Andosols, Arenosols, Chernozems, Calcisols, Fluvisols, Luvisols, Lixisols, Phaeozems, and Vertisols after correcting soil profiles in -4.8, -0.2, -0.7, -1.1, -0.2, -0.9, -0.9, -0.2, -0.4, and -0.1%, respectively. These soils are characterized for their higher fertility than previous group of soils. The potential cause of reduced simulated yields in high fertility soils, whereas increased simulated yields in low fertility soils after the soil profile reanalysis, can be due to the default values used by the crop model to fill the missing values, which apparently are over and under estimated respectively on each group of soils. In some locations, differences in simulated crop yields reached values as high as 41.5% on Gleysols in the Phillipines, and 22.5% on Acrisols in Thailand.

5. Conclusions

The WISE v 1.1 soil database was subjected to a quality control procedure to correct inconsistencies in soil property values and to estimate missing values. The overall goal was to correct and recover data where possible, because improper handling of data could have distorted an original soil analysis. Soil parameters that showed a high number of discrepancies were pH determined in water, pH determined in buffer, cation exchange capacity, and hydraulic conductivity. Estimation of missing values was focused on soil organic carbon and soil nitrogen. 70%, or 1647, soil nitrogen missing values were estimated applying the C/N ratio rule. There were a low number of missing values for soil organic carbon. Overall, 34 soil profiles out of 748 with missing organic carbon values were estimated, which represented just 5% of the total. Missing values were not estimated for microelements, phosphorus and sulfur in these soils.

The comparison of the CSM-CERES-Maize model simulations with both the original and the improved datasets gave 1294 soil profiles with different crop yield outputs, representing 38% of the WISE v 1.1 soil database. The CSM-CERES-Maize model worked successfully with all the soil profiles from the new global soil database for crop and environmental modeling.

In most cases missing values were not estimated and discrepancies were left as they are. Modifications were made carefully with the intention to make valid soil information for modeling applications in agriculture, not to replace an established standard soil profile description. Note that some soil profiles descriptions in the WISE database could include non-agricultural soils; however, a non-agricultural soil profile is a potential agricultural soil for a user in need of some information for a determined area. There are still some uncertainties related to both the corrected and estimated data, as well as the original soil database. Several soil parameters are characterized by their *in situ* variability as a response to the farming practices, weather, season, etc. Therefore, users need to be careful with some of the data and be aware of these limitations.

Acknowledgments

This project was supported through a grant between the International Food Policy Research Institute (IFPRI) and the University of Georgia under the auspices of the U.S. Agency for International Development (AID)-Consultative Group on International Agricultural Research (CGIAR) Linkage Fund. Support was also provided by the Harvest Choice Project.

The efforts of the International Soil Reference and Information Centre (ISRIC) to develop the World Inventory of Soil Emission Potential (WISE) database are duly recognized.

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