The relations between soil water retention characteristics, particle size distributions, bulk densities and calcium carbonate contents for Danish soils

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Abstract A database containing about 800 soil profiles located in a 7-km grid covering Denmark has been used to develop a set of regression equations of soil water content at pressure heads −1, −10, −100 and −1500 kPa versus particle size distribution, organic matter, $CaCO_3$ and bulk density. One purpose was to elaborate equations based on soil parameters available in the Danish Soil Classification's texture database of particle size distribution and organic matter. It was also tested to see if inclusion of bulk density or $CaCO_3$ content (in $CaCO_3$-containing samples) as predictors or grouping in surface and subsurface horizons or textural classes improved the regression equations. Compared to existing Danish equations based on much fewer observations the accuracies of the new equations were better. The equations also predicted the soil water content at the measured pressure heads more accurately than the pedotransfer functions developed in HYPRES (Hydraulic Properties of European Soils). Introducing bulk density as a predictor improved the equation for the pressure head of −1 kPa but not for the lower ones. The grouping of data sets in surface and subsurface horizons or in textural classes did not improve the equations. Based on the equations a set of van Genuchten parameters for soil types in the Danish Soil Classification was elaborated. The prediction of soil water content, especially at pressure head −1 kPa, is more accurate using these van Genuchten parameters than using the pedotransfer functions developed in relation to the HYPRES database from a broad range of European soils.

Keywords Pedotransfer functions; soil databases; soil texture; soil water retention

Introduction

Hydraulic characteristics are important properties of soils in relation to water planning. Basic characteristics are the soil water retention curve and the hydraulic conductivity as a function of soil water content or matrix potential. Measurements of hydraulic properties are expensive and time consuming, and they have not been measured as routine concurrent with basic soil parameters during soil mappings in Denmark. Therefore, functions have been developed in the past to relate basic soil data such as texture, organic matter content and bulk density to soil hydraulic properties. Such functions are known as pedotransfer functions (PTFs) (Bouma 1989) and at least two different kinds of PTFs can be distinguished. One predicts water content at specific pressure heads. Such equations have been reported, for example, by Gupta and Larson (1979) and Ahuja *et al.* (1985) and studies performed in the Nordic countries have been reviewed by Riley *et al.* (1990). Other kinds of PTFs are continuous functions of soil water retention and hydraulic conductivity in relation to water content. The PTFs then relate basic soil data to factors shaping the hydraulic functions. Examples of such PTFs have been presented by Rawls *et al.* (1982) based on soils from the USA, by Rajkai *et al.* (1996) based on Swedish soils and by Wösten *et al.* (1999) based on a broad range of soils from Europe. Reviews of the development of PTFs are presented, for example, by Rawls *et al.* (1991)

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and Wösten *et al.* (2001). Which PTF to use in modelling in a specific region depends on a) which hydraulic information is needed, b) which soil parameters are available in relation to soil parameters that the potential PTFs require and c) which of the potential PTFs have been developed from soils with the best representativity of the soils in the region in question.

In Denmark former PTFs have been elaborated to predict the available soil water for plants for calculations of irrigation need based on texture data from Danish soil maps. The PTFs used were regression equations expressing the soil water content at pressure heads −10 and −1500 kPa by weight percentages of clay, silt, fine sand and organic matter content picked from soil data from Nothern Jutland (Madsen and Platou 1983). Similar equations had also been published based on soil data from 15 Danish agricultural research stations (Hansen 1976) and from soils from Southern Jutland (Madsen 1986). These investigations included soils of different geological origins and pedological development, but the datasets were limited in number and they only represent a limited part of the variations in geological deposits and pedological development found in Denmark.

Today, water planning often involves hydraulic simulation models, which require continuous functions of soil water retention characteristics and hydraulic conductivity in relation to water content. In Denmark, a soil–plant–atmosphere simulation model called DAISY has been developed (Hansen *et al.* 1990) and recently an user-friendlier version called DaisyGIS (DHI–Water and Environment 2001) has been released. Using those models in Denmark, PTFs relating existing basic soil data to hydraulic properties often have to be used and in DaisyGIS, for example, three sets of PTFs are built-in based on US, Belgian or European soil data. When modelling under Danish conditions the most obvious choice of PTFs in DaisyGIS are those developed for the HYPRES (Hydraulic Properties of European Soils) database because they are based on soil data from Europe including Denmark. These PTFs are related to Mualem–van Genuchten parameters (Wösten *et al.* 1999). As an input to the PTFs the most comprehensive source of measured basic soil data in Denmark is the texture database related to the Danish Soil Classification (Larsen and Sørensen 1996). But when using these data two questions arise: a) how to estimate bulk density, which is included in the HYPRES PTFs but is not measured in relation to the Danish Soil Classification and b) how well does the HYPRES PTFs represent Danish soil conditions?

The establishment of a database containing pedological soil profile data sampled in a 7-km grid covering Denmark provides a new basis for developing PTFs. The database contains analyses of soil water retention characteristics, particle size distributions (PSD), organic matter (OM), $CaCO_3$ content and bulk density (BD) (Madsen and Jensen 1996). This database includes approximately 800 soil profiles and gives a good statistical representation of Danish soils due to the systematic sampling, its relatively many observations and because it covers the whole country. In this paper it is investigated if PTFs developed from the pedological soil database and using the same soil parameters, which are stored in the Danish Soil Classification texture database, can improve existing PTFs for modelling in Denmark. For that a set of regression equations have been produced expressing soil water content at pressure heads −1, −10, −100 and −1500 kPa from soil data which are available in the Danish Soil Classification texture database. In addition the effect of including BD in the equations, even though this information is not available in the Danish Soil Classification texture database, is also investigated. The equations found are compared to existing Danish equations and to the HYPRES PTFs prediction of soil water content at the investigated pressure heads. For the estimation of BD, which has to be used in the HYPRES PTFs, a regression equation expressing BD vs PSD and OM is developed from the pedological soil database as well. As an example of their application the regression equations are used as a step towards predictions of average Mualem–van Genuchten parameters for soil types in the Danish Soil Classification.

Materials and methods

Deposits and soils in Denmark

The Danish landforms were mainly formed during the Saale and Weichsel glaciation eras and the Holocene. Glacial deposits from Weichsel, mainly loamy and sandy tills, cover most of the country. In many tills, $CaCO_3$ has been incorporated from high-lying Cretaceous and Danien limestones. Since being deposited, acid rain and acidification processes in the soils have dissolved and washed out the $CaCO_3$ from the topsoil. In many soil profiles in the eastern part of the country, $CaCO_3$ is still found in lower horizons, where it can make up 30–40 wt% of the till. In Western Jutland the Saale glaciation landscapes are found to be influenced by periglacial processes during Weichsel and cut through by outwash plain deposits during Weichsel. In Northern Jutland marine deposits cover large areas and along the West Coast of Jutland sand dunes and salt marsh deposits dominate. The soil forming processes on well-drained sites in Denmark are a) acidification due to leaching of $CaCO_3$ and exchangeable bases, b) weathering of minerals, c) migration of clay particles on loamy soils and d) podzolisation of sandy soils. In wetlands, gley processes and peat formation are dominant soil forming processes. The occurrence of the main soil types is shown in Table 1.

Soil databases

In 1986 the Danish Agricultural Advisory Centre established a nationwide 7-km grid of soil profiles aimed at advising farmers according to the soils' optimal nitrogen fertilisation (Østergård 1990). More than 800 sites were located from the grid's intersections and of these about 660 were located on farmland, slightly more than 100 in forests and the rest on other types of land use. Soil profile investigations were carried out as close to the grid intersections as possible (Madsen and Jensen 1996) and bulk soil samples were extracted from each major soil horizon and analysed in the laboratory for chemical and physical properties. Additionally, three undisturbed soil samples from each horizon were extracted in steel rings of about 100 cm^3 for soil water retention determinations. The following particle sizes were determined: <2 μm, 2–20 μm, 20–63 μm, 63–125 μm, 125–200 μm, 200–500 μm and 500–2000 μm. Furthermore OM, the content of $CaCO_3$ and BD were determined. In the pedological soil profile database the particle sizes, OM and $CaCO_3$ are given as wt% of the total sum of particle sizes, OM and $CaCO_3$. BD is given as g/cm^3. The laboratory methods are described in Madsen and Jensen (1992).

In relation to the Danish Soil Classification a soil texture database had been established from analyses of soil samples from more than 32 000 locations all over the country. At each location soil samples were taken from a depth of 0–20 cm and from around 1/7 of the locations a sample from the subsoil was also taken, normally from a depth of 35–55 cm. The following particle sizes were determined: <2 μm (Cl), 2–20 μm (fSi), 20–63 μm (cSi), 63–200 μm (fSa) and 200–2000 μm (cSa). Additionally, OM and the content of $CaCO_3$ were determined. The parameters are given as wt% of the sum of the weight of the particles and OM. The database was established together with soil maps at 1:50 000 scale showing soil types classified relative to the soil texture of the upper 20 cm of soil. The soil types were

Table 1 Distribution in % of soil types in Denmark according to FAO-Unesco (1990)

PZ	AR	AL, PD	LV	CM	GFH	LP
20–30	10–20	0–10	20–30	10–20	10–20	0–10

PZ: Podzol; AR: Arenosol; AL,PD: Alisol and Podzoluvisol; LV: Luvisol and Phaeozem with clay illuviation; CM: Cambisol and Phaeozems without clay illuviation; GFH: Gleysol, Fluvisol, Histosol; LP: Leptosol. (After Madsen and Jensen 1996.)

called Map Colour Codes (MCC) and Table 2 show the definition of MCC1-5, which covers 94% of the mapped area.

Regression analysis

All regression analyses were carried out using the linear regression analysis facilities available in the SPSS software for Windows v. 11.0 and SAS v. 8.2. Before the statistical analysis some samples with special physical and chemical properties for soil were excluded. Those were all samples with more than 10% OM and samples with BD lower than 1.0 g/cm^3. These samples were mainly found in soil horizons from wetlands. Furthermore, $CaCO_3$-containing samples were excluded except from till deposits. This left up to 2423 observations for a forward stepwise regression analysis where the dependent variable was the soil water content at each of the pressure heads −1, −10, −100 and −1500 kPa and the predictors were OM and PSD and for some tests also $CaCO_3$ and BD (for units, see the next paragraph). The regression equations tested are:

$$\theta_{\mathrm{h}} = (a \times \mathrm{OM}) + (b \times \mathrm{Cl}) + (c \times \mathrm{fSi}) + (d \times \mathrm{cSi}) + (e \times \mathrm{fSa}) + (f \times \mathrm{cSa}) + \mathrm{constant} \quad (1)$$

$$\theta_{\mathrm{h}} = (a \times \mathrm{OM}) + (b \times \mathrm{Cl}) + (c \times \mathrm{fSi}) + (d \times \mathrm{cSi}) + (e \times \mathrm{fSa}) + (f \times \mathrm{cSa}) + (g \times \mathrm{BD}) + \mathrm{constant} \quad (2)$$

$$\theta_h = (a \times \mathrm{OM}) + (b \times \mathrm{Cl}) + (c \times \mathrm{fSi}) + (d \times \mathrm{cSi}) + (e \times \mathrm{fSa}) + (f \times \mathrm{cSa}) + (h \times \mathrm{CaCO_3}) + \mathrm{constant} \quad (3)$$

where θ_{h} is the percent soil water content by volume at pressure head h and a–h are regression coefficients.

Each equation was tested for each pressure head. Equations (1) and (2) were tested using all datasets, while Eq. (3) was tested on $CaCO_3$-containing samples only. Equation (1) was also tested if better equations in terms of higher r^2 values were obtainable after grouping the data into surface and subsurface horizons and into texture classes of the Danish Soil Classification. In that way 40 equations were tested from which the most significant will be presented.

Data transformations and calculations

Before the regression analyses the particle size classes in the pedological database were transformed to match those found in the Danish Soil Classification texture database by adding the particle classes 63–125 μm, 125–200 μm, 200–500 μm and 500–2000 μm to 63–200 μm and 200–2000 μm. Also the wt% units of particle sizes, OM and $CaCO_3$ in the pedological soil profile database were transformed to be given in terms of the percent of the weight of the particle sizes and OM, as in the Danish Soil Classification texture database.

Table 2 Definitions of soil types MCC1–5 in the Danish Soil Classification

Map colour code (MCC)	Soil type	Percentage by weight: Clay <2 μm	Silt 2–20 μm	Fine sand 20–200 μm	Total sand 20–2000 μm	Organic matter
1	Coarse sand	0–5	0–20	0–50	75–100	<10
2	Fine sand	0–5	0–20	50–100	75–100	< 10
3	Clayey sand	5–10	0–25	0–95	65–95	< 10
4	Sandy clay	10–15	0–30	0–90	55–90	< 10
5	Clay	15–25	0–35		40–85	< 10

As a measure of the accuracy of the equations the root mean square error (RMSE):

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{1}^{N} (y_m - y_p)^2}{N}} \tag{4}$$

is used, where y_m and y_p are the measured and predicted values.

The HYPRES PTFs relates OM, clay (<2 μm), silt (2–50 μm) (wt% in relation to the minerogene fraction) and BD (g/cm^3) to the parameters (θ_s, α and n) of the closed form Mualem-van Genuchten equation (van Genuchten 1980):

$$\theta\ (\psi) = \theta_r + \frac{(\theta_s - \theta_r)}{[1 + (\alpha\psi)^n]^m} \tag{5}$$

where ψ = soil matrix potential (cm), θ = soil moisture content, θ_r = residual water, θ_s = saturated moisture content, and α, n and m are curve shaping factors where m is assumed equal to 1-1/n. The soil water content had been calculated at pressure heads − 1, − 10, − 100 and − 1500 kPa given the assumption that θ_r = 0.025 for coarse textured soils (clay < 18% and sand > 65%) and θ_r = 0.01 for finer textured soils.

In this work the accuracy of the HYPRES PTFs are tested in the situation of having no measurements of BD, which is the case when using the information from the Danish Soil Classification database. In that case a value of BD has to be estimated and that is done using a regression equation based on the pedological database:

$$\mathrm{BD} = -(0.068 \times \mathrm{OM}) - (0.002 \times \mathrm{Cl}) - (0.005 \times \mathrm{fSi}) - (0.007 \times \mathrm{cSi}) - (0.005 \times \mathrm{fSa}) - 0.006 \times \mathrm{cSa}) + 2.157 \tag{6}$$

where r^2 = 0.45 and n = 2431. Before using the HYPRES PTFs the silt class in the database was redefined from 2–20 μm and 20–63 μm to 2–50 μm using an interpolation method based on a Gaussian distribution function and the wt% units were transformed to be in percent of the weight of the minerogene fraction.

For prediction of the Mualem–van Genuchten parameters θ_r, θ_s, α and n for the soil types in the Danish Soil Classification the non-linear least-squares optimization program RETC (van Genuchten *et al.* 1991) was used.

Results and discussion

Regression coefficients for equations relating soil water content at different pressure heads and OM and PSD corresponding to the parameters stored in the Danish Soil Classification database are presented in Table 3, Eq. (1). The coefficient values show the importance of OM to the soil water content in the equations but also the increasing importance of clay at decreasing pressure heads, which are also the general findings in other Scandinavian studies, as summarized by Riley *et al.* (1990). The r^2 value for pressure head − 1 kPa is relatively low. The water content at this pressure head is not only influenced by the OM and PSD but also by BD (Reeve *et al.* 1973; Riley *et al.* 1990). If BD is included as a predictor it improves the r^2 value of the equations for − 1 kPa, Table 3, Eq. (2), but not for pressure head − 10 kPa and only negligibly for pressure heads − 100 and − 1500 kPa. In many till-rich subsoils in Denmark the content of $CaCO_3$ is from fragments of limestone in the form of powder and clasters. Including $CaCO_3$ content as a predictor in the regression analysis performed on $CaCO_3$-containing samples resulted in equations with higher r^2 values for water content at pressure heads − 1 and − 10 kPa compared to equations without lime content as a predictor, Table 3, Eq. (3). For the lower pressure heads the equations were independent of the $CaCO_3$ content.

Table 3 Regression coefficients for Eqs. (1)–(3), see text, at various pressure heads

Eq. no.	θ_h (kPa)	OM	Cl	fSi	cSi	fSa	cSa	BD	$CaCO_3$	Const.	r^2	*n*
Eq. (1)	−1	2.25	0	−0.11	0	0	−0.03	*	*	35.86	0.40	2423
Eq. (1)	−10	2.64	0.39	0	0.23	−0.04	−0.16	*	*	20.33	0.83	2423
Eq. (1)	−100	1.83	0.69	0.25	0.16	0.02	0	*	*	0.81	0.86	2420
Eq. (1)	−1500	0.64	0.51	0.04	0.03	0	0	*	*	−0.50	0.90	2333
Eq. (2)	−1	0.47	0.09	0	0	0.03	−0.01	−27.38	*	76.83	0.78	2423
Eq. (3)	−1	2.04	0.21	0.12	0	0	0	*	−0.21	29.28	0.44	171
Eq. (3)	−10	0.89	0	0	0	−0.24	−0.35	*	−0.13	42.71	0.74	171

*Parameter not included in the regression analysis

It was tested if a distinction between topsoil and subsoil or a distinction between textural classes according to the soil types in the Danish Soil Classification before regression analysis would improve the equations. But none of these equations turned out to have a higher r^2 value than the equations based on the total dataset.

Comparisons with existing equations

The accuracy of the new vs the old equations from Denmark is shown in Table 4 as the root mean square error between measured and predicted values, Eq. (4). The accuracy of the equations is higher the lower the pressure heads. The errors of the former Danish equations are larger than the new ones. This might be the result of the limited amount of soil data used when developing the former equations compared to the new. To calculate the accuracy of the HYPRES PTFs the soil water content of the four pressure heads was calculated from the Mualem–van Genuchten equation, Eq. (5), using the predicted van Genuchten parameters and these values were compared with the measured values. The predictions of water content were based on the measured value of BD in the dataset as well as on the predicted value of BD using Eq. (6). In both cases the errors of the HYPRES equations are larger than the new equations; especially for −1 kPa using the predicted BD. In the literature, typical values of RMSE from PTFs lie between 3–5 for −10 kPa and 2–7 for −1500 kPa and normally the accuracy of those equations predicting a complete retention curve is lower than when specific pressure heads are predicted (Wösten *et al.* 2001). The lower accuracy of the HYPRES PTFs in this comparison might also be explained by the fact that these functions are based not only on Danish soils but on a wide range of European soils.

Prediction of average hydraulic parameters for soil types in The Danish Soil Classification

As an example of their application, the equations found are used to predict van Genuchten parameters for soil types (MCC1–5) in the Danish Soil Classification in topsoils as well as subsoils. From the texture database related to the Danish Soil Classification, average OM and PSD are calculated for topsoil and subsoil based on samples from 0–20 cm and 35–55 cm depths, respectively, after classifying the samples according to the soil type definitions in Table 2. From this information the average soil water content for the pressure heads −1, −10, −100 and −1500 kPa were calculated using Eq. (1) and the regression coefficients in Table 3. The soil water content at the four pressure heads has further been used to predict the van Genuchten parameters θ_r, θ_s, α and n from RETC, Table 5. To use this data as input parameters in DaisyGIS a value for the saturated hydraulic conductivity, K_s, is also required. However, K_s is not measured in relation to the pedological soil database, but an estimation from OM and PDS can be predicted using HYPRES PTFs given in Wösten *et al.* (1999)

Table 4 Root mean square error of the predicted values of water content from new and former equations compared to measured values (% water content by vol.)

Equation	−1 kPa	−10 kPa	−100 kPa	−1500 kPa
Eq. (1)	3.9	3.8	2.9	1.3
Eq. (2)	2.4			
Hansen (1976)				2.3
Madsen and Platou (1983)		4.3		1.7
Madsen (1986)		4.7		3.7
HYPRES (measured BD)	4.4	4.4	4.4	2.1
HYPRES (predicted BD)	5.7	4.4	3.9	2.2

Table 5 Calculated van Genuchten parameters and K_s for topsoil and subsoil for the soil types MCC1–5 of the Danish Soil Classification. θ_r: initial values from RETC; θ_s, α and n: calculated from RETC based on predicted values of water content from the new regression equations; K_s predicted from HYPRES PTFs (BD calculated by Eq. (6))

MCC	USDA	Sample depth (cm)	θ_r	θ_s	α (1/cm)	n	K_s (cm/d)
1	Sand	0–20	0.045	0.4705	0.0671	1.4621	139.8
2	Loamy sand	0–20	0.057	0.4468	0.0264	1.5631	104.7
3	Sandy loam	0–20	0.065	0.4374	0.0275	1.4448	73.4
4	Sandy loam	0–20	0.065	0.3949	0.0171	1.3596	41.3
5	Sandy loam	0–20	0.065	0.3889	0.0038	1.4101	34.6
1	Sand	35–55	0.045	0.4433	0.0731	1.6105	91.1
2	Sand	35–55	0.045	0.4189	0.0316	1.6230	66.3
3	Sandy loam	35–55	0.065	0.4051	0.0320	1.5173	44.6
4	Sandy loam	35–55	0.065	0.3691	0.0203	1.3750	25.2
5	Sandy loam	35–55	0.065	0.3639	0.0089	1.3194	16.7

(BD calculated from Eq. (6)), which is also presented in Table 5. For comparison, the classifications of the average textures of MCC1–5 according to USDA (Soil Conservation Service 1975) are shown. In Table 6 are shown the average values for the textural groups according to USDA of the van Genuchten parameters θ_s, α and n (Carsel and Parrish 1988). The values of θ_r are the initial values in RETC for the texture classes and they are the same in both investigations. As both sets of van Genuchten parameters express average values of texture classes, which are different in their definition, they are not likely to be the same value. Compared to those presented by Carsel and Parrish (1988), the value of θ_s from this paper is relatively high for texture class sand, the α value is relatively high for all three texture classes but the n value is lower for all three texture classes.

Predicted soil water contents for MCC1–5 topsoils and subsoils respectively using the van Genuchten parameters in Table 5 and the predicted soil water contents using HYPRES (BD calculated from Eq. (6)) are compared with the average measured soil water contents in terms of RMSE, Table 7. The prediction of soil water contents from van Genuchten parameters found by the new regression equations and RETC give a better prediction for pressure head −100 and especially for −1 kPa compared to the prediction from HYPRES PTFs. The opposite is the case for pressure head −1500 kPa but to a lesser degree. As the coarse pores of the soil matrix account for more water transport than the small pores in the wet season during autumn, winter and spring, this may indicate that hydraulic properties predicted by the new equations and RETC on average give a better basis for simulating water flow than using the HYPRES PTFs, which is built-in in, for example, DaisyGIS, when soil data is limited to those found in the Danish Soil Classification texture database. But this has to be examined by testing the model in practice.

Table 6 Average values for the textural groups according to USDA of the van Genuchten parameters θ_r, θ_s, α and n (Carsel and Parrish 1988)

USDA	θ_r	θ_s	α (1/cm)	n
Sand	0.045	0.43	0.145	2.68
Loamy sand	0.057	0.41	0.124	2.28
Sandy loam	0.065	0.41	0.075	1.89

Table 7 Root mean square error of predicted values of water content (in % water content by vol.) compared to average measured values of topsoils and subsoils of soil types MCC1–5. Predicted values are calculated from the Mualem–van Genuchten equation, Eq. (5), using the van Genuchten parameters in Table 5 and from HYPRES PTFs based on average texture and OM content of the soil types (BD calculated by Eq. (6))

van Genuchten parameters from	−1 kPa	−10 kPa	−100 kPa	−1500 kPa
Table 5	0.8	2.7	1.5	2.8
HYPRES	3.0	2.7	3.2	1.5

Conclusions

Relatively good regression equations are found for soil water content at pressure heads −10, −100 and −1500 kPa versus basic soil information in the form of particle size distribution and content of organic matter. Including bulk density as a predictor improve the equation for soil water content at pressure head −1 kPa, but not for the lower pressure heads also investigated.

Distinguishing between topsoil and subsoil or between the soil types MCC1–5 defined in the Danish Soil Classification did not improve the equations compared to equations based on all samples.

Prediction of water content in lime-containing till can be improved in terms of the r^2 value for pressure head −1 and −10 kPa by using the equation including lime content as a predictor compared to the equations excluding this parameter, but not for the lower pressure heads also investigated.

The new equations give better predictions than the former Danish ones probably because the representativity of the soil data used when developing the equations is better.

It seems possible to develop more precise PTFs for van Genuchten parameters from the Danish pedological soil profile database than the existing PTFs developed in relation to the HYPRES database from a wide range of European soils for use with the Danish Soil Classification's texture database.

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