Implementation of a method for converting soil properties into building physical material properties

Grunewald, John\textsuperscript{1,}\textsuperscript{*}; Hirsch, Hauke\textsuperscript{1}; Petzold, Hans\textsuperscript{1}

\textsuperscript{1}Dresden University of Technology, Institute of Building Climatology, 01060 Dresden, Germany

Abstract. This article presents a method that can be used to convert soil properties into building physical material properties that meet the requirements of modern codes for transient hygrothermal simulations. The soil input data must be specified by the so-called “van Genuchten parameters” in order to predict the water retention curve and the hydraulic conductivity of unsaturated soils. The percentages of silt, sand and clay are used to calculate the moisture-dependent thermal conductivity for soils with different water saturation. The output is a validated set of hygrothermal material functions (moisture storage function, liquid water conductivity, water vapour conductivity, thermal conductivity), which is prepared for use in simulation projects or for inclusion in a database. The methodology described in this document has been implemented in an MS Excel tool that enables an efficient, almost fully automatic conversion of a list of soils in three steps.

1 Introduction

In the cities of Schleswig and Bad Nauheim, Germany, residential pilot projects are being developed that use what is known as near-surface geothermal energy in combination with cold district heating networks (non-insulated earth pipes) to supply heating to the settlements. In winter, heating energy is obtained from geothermal collectors at a depth of 2-5 m, which enables the soil to be thermally regenerated by the climate. Part of the strategy is to freeze the soil in winter, use the latent heat of the freezing process as additional heating energy and provide sufficient cooling energy in summer. One of the goals is to promote maximum bidirectional energy shift between seasons. Several accompanying research projects\textsuperscript{ab} funded by the German Federal Ministry for Economic Affairs and Energy (BMWi) are carried out to understand and optimize these systems.

One of the research questions is how to adequately characterize the hygrothermal material properties of soils. The material characterization should match the requirements of modern simulation tools and the procedure should be quick, save and easy to use. Therefore, a tool has been developed that can automate major parts of the procedure. Since Microsoft Excel is widely used and can be operated by almost everyone, it was decided to build the tool upon this basis. The functions are implemented as macros and the software is called “SoilGenerator”.

In this paper, the creation of parameterized soils for DELPHIN\textsuperscript{c} applications will be introduced in following steps:

- Generation of moisture-dependent thermal conductivity function,
- Optimization of the DELPHIN-GAUSS function for moisture storage,
- Conversion of the water retention function / hydraulic conductivity,
- Creation and export of a material file (*.m6).
- Determination of the water absorption coefficient by simulation of the water suction experiment,

The data sources listed below have been used:

- Van Genuchten parameters \cite{1} of the water retention function / hydraulic conductivity given in \cite{2},
- Water content / density / thermal conductivity / heat capacity according to \cite{3},
- Estimation of diffusion resistances using reference materials from DELPHIN-MatDB.

The developed conversion procedure is applied to the most common soil types as classified according to their silt, sand and clay percentages in \cite{4}, which are Sand, Loamy Sand, Sandy Loam, Loam, Silt, Silty Loam, Sandy Loam, Sand, Loamy Sand, Sandy Loam, Loam, Silt, Silty Loam, Sandy

\textsuperscript{a} ErdEis1 - Joint Research Project: Soil Ice Storage and Near-surface Geothermics (Fundamentals), Project file number 03ET1382A, Project duration 01.04.2016 - 31.08.2018, https://projektinfos.energiewendebauen.de/foerderkennzeichen/03et1382a

\textsuperscript{b} ErdEisII - Joint Research Project: Soil Ice Storage and Near-surface Geothermics (Implementation), Project file number 03ET1634C, Project duration 01.03.2019 - 28.02.2022, https://projektinfos.energiewendebauen.de/foerderkennzeichen/03et1634c

\textsuperscript{c} DELPHIN6 – A Simulation program for the calculation of coupled heat, moisture, air, pollutant, and salt transport, https://bauklimatik-dresden.de/delphin/index.php?la=en

\textsuperscript{*} Corresponding author: john.grunewald@tu-dresden.de

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Clay Loam, Clay Loam, Silty Clay Loam, Sandy Clay, Silty Clay, and Clay (see Fig 1).

Fig 1. USDA classification of soils [5], source: http://epidote.wvgs.wvnet.edu/enviro/lab5.html

2 Input data evaluation

The silt, sand and clay percentages \( p_{\text{silt}}, p_{\text{sand}} \) and \( p_{\text{clay}} \), as well as the van Genuchten parameters \( \theta_{\text{res}}, \theta_{\text{sat}}, \alpha, n \) and \( K_{\text{sat}} \) of the soils must be given as shown in Table 1. The SoilGenerator software parses through all rows of the table and performs the respective conversion operations.

The silt, sand and clay percentages are the basis for calculation of the moisture dependent thermal conductivity \( \lambda(\theta) \) after a model from [6], eq. (1). The van Genuchten model [1], eq. (2) - (3) is used to generate the water retention curve \( \theta(S_e) \) and the hydraulic conductivity \( K(\theta) \). The secondary quantities are relative (normalized) thermal conductivity \( \lambda_r(\theta) \), the saturation degree \( S_e(\psi) \), the matrix potential \( \psi(p_c) \), and the relative hydraulic conductivity \( K_r(\theta) \).

\[
\lambda(\theta) = (\lambda_{\text{sat}} - \lambda_{\text{dry}}) \cdot \lambda(\theta) / \theta_{\text{sat}} + \lambda_{\text{dry}}
\]

\[
\theta(\psi) = (1 + (\alpha \cdot \psi)^n)^{-m} ; m = 1 / n
\]

\[
\theta(p_c) = p_c / (\rho \cdot g)
\]

\[
K(\theta) = K_{\text{sat}} \left[ 1 - (1 - \theta_{\text{sat}}^{-1})^n \right]^2
\]

The respective parameters and constants are:

- \( \theta_i \) Liquid water content in m\(^3\)/m\(^3\)
- \( \theta_{\text{res}} \) Residual water content in m\(^3\)/m\(^3\)
- \( \theta_{\text{sat}} \) Saturation water content in m\(^3\)/m\(^3\)
- \( \alpha \) Horizontal curve shift parameter in 1/cm
- \( n \) Slope parameter
- \( K_{\text{sat}} \) Saturated hydraulic conductivity in cm/h
- \( p_c \) Capillary pressure in Pa
- \( \rho \) Density of liquid water (=1000 kg/m\(^3\))
- \( g \) Gravity constant (=9.81 m/s\(^2\))
- \( pC \) Log. capillary pressure (=0…10) log(Pa)
- \( \lambda_{\text{dry}} = 0.026; \lambda_{\text{water}} = 0.556 \text{ W/m K} \)
- \( \lambda_{\text{silt}} = 3.5; \lambda_{\text{sand}} = 4.5; \lambda_{\text{clay}} = 2.5 \text{ W/m K} \)

<table>
<thead>
<tr>
<th>Soil</th>
<th>( p_{\text{silt}} )</th>
<th>( p_{\text{sand}} )</th>
<th>( p_{\text{clay}} )</th>
<th>( \theta_{\text{res}} )</th>
<th>( \theta_{\text{sat}} )</th>
<th>( \alpha )</th>
<th>( n )</th>
<th>( K_{\text{sat}} )</th>
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<td>0.43</td>
<td>0.145</td>
<td>2.68</td>
<td>29.700</td>
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<td>0.43</td>
<td>0.124</td>
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<td>0.41</td>
<td>0.075</td>
<td>1.89</td>
<td>4.421</td>
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<td>0.2</td>
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<td>0.46</td>
<td>0.016</td>
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<td>0.02</td>
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<td>0.27</td>
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<td>0.39</td>
<td>0.059</td>
<td>1.48</td>
<td>1.308</td>
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<td>0.43</td>
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<td>0.41</td>
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<td>0.38</td>
<td>0.008</td>
<td>1.09</td>
<td>0.200</td>
</tr>
</tbody>
</table>
For Silt, the results of the calculation of the respective material functions are shown in Fig 2 - Fig 4.

**Fig 2.** Thermal conductivity of Silt.

**Fig 3.** Water retention curve of Silt.

**Fig 4.** Hydraulic conductivity of Silt.

**Fig 5.** Moisture storage function of Silt.

### 3 Approximation of the moisture storage function

Normally, soils never become completely dry or at least this case is probably not of interest to soil physicists. In building physics, the situation is different. Building materials should usually stay dry to avoid moisture damage. Therefore, the residual water content is not used in building physics and is no material parameter in DELPHIN. Instead, the sorption isotherm \( \theta(pC) \) is experimentally determined to characterize the moisture storage in building materials at low water (or moisture) contents in terms of relative humidity. The moisture storage function \( \theta(pC) \) in building physics combines the water retention curve (overhygroscopic range) and the sorption isotherm (hygroscopic range). Both functions are connected through an equilibrium assumption between the liquid and vapour phases in the building material expressed by the Kelvin equation (5).

\[
p_{lc}(\varphi) = -\rho \cdot R \cdot T \cdot \ln(\varphi)
\]

\( \varphi \)  Relative humidity  
\( R_v \)  Specific gas constant of water vapour (=462 J/kgK)  
\( T \)  Temperature in K

The usage of the water retention curve \( \theta(Se) \) "as it is" causes two problems: 1) the constant values in the range \( pC=[0...2] \) create an ill-posed problem (small changes of water content result in big changes of capillary pressure) and 2) there is a residual water content \( \theta(\varphi=0)=\theta_{res} \).

Therefore, the water retention curve is approximated by a three-modal GAUSSIAN normal distribution ensuring a steadily decreasing course of the moisture storage function. Equation (6) is the pore volume distribution and its integral (7) is the moisture storage function.

\[
\frac{d\theta_i}{dpC} (pC) = \sum_{i=1}^{N} \frac{\Delta \theta_{li}}{\sqrt{2\pi} \cdot S_i} \cdot \exp \left( \frac{(pC_i - pC)^2}{2 \cdot S_i^2} \right)
\]

\[
\theta_i (pC) = \sum_{i=1}^{N} \frac{\Delta \theta_{li}}{2} \cdot \left( 1 + \text{erfc} \left( \frac{pC_i - pC}{\sqrt{2} \cdot S_i} \right) \right)
\]

\( N \)  Modality (=3)  
\( pC_i \)  Peak values in pore volume distribution  
\( S_i \)  Standard deviations  
\( \Delta \theta_{li} \)  Differential plateau values
The first modality is used to model the curve in the saturated range \( pC=\{0...2\} \), the second modality approximates the water retention curve in the overhygroscopic range \( pC=\{2...5\} \) and the third modality models a sorption isotherm in the hygroscopic range \( pC=\{5...10\} \). The approximation of the moisture storage function of Silt by application of the least square method (using the Excel solver) is shown in Fig 5.

The values of the water retention curve generated from the van Genuchten parameters are only used in the overhygroscopic range (plotted by red dots). The optimized moisture storage function is given in the whole moisture range as indicated by the blue solid line.

With the determined parameters of the moisture storage function, the courses of the sorption isotherm (Fig 6) and of the pore volume distribution (Fig 7) can be easily derived.

\[
\sum_{i=1}^{N} \Delta \theta_{i,j} = \theta_{\text{eff}} \tag{8}
\]

In order to avoid convergence errors during numerical simulation caused by ill-posed problems, the mathematical optimization of the moisture storage function should include additional constraints. For example, the standard deviations can be limited not to fall below a minimum such that a continuous pore spectrum is received. The additional constraints (9) avoid flat plateaus in the moisture storage function and provide a continuously decreasing function.

\[
S_l > S_{\text{min}} \rightarrow \frac{d\theta_{\text{sat}}}{dpC(pC)} > 0 \tag{9}
\]

The derived moisture storage function \( \theta(pC) \) is used to generate a data set of 101 equidistant value pairs for the range of \( pC=\{0...10; \text{ step 0.1}\} \), which is exported to the DELPHIN6 material file.

### 4 Generation of the liquid water conductivity

The liquid water conductivity \( K_l(\theta) \) in (10) is defined slightly differently than the hydraulic conductivity \( K_h(\theta) \) in (11). In building physics, the liquid mass flux density \( j_l \) in kg/m²s is associated with the gradient of the capillary pressure \( \nabla p_c \) while in soil physics the liquid volumetric flux density \( v_l \) in m³/m³s is connected with the gradient of the matrix potential \( \nabla h \). Note that the volumetric flux density corresponds to a velocity.

\[
j_l = -K_l \cdot (\nabla p_c + \rho_l g) \tag{10}
\]

\[
v_l = -K_h \cdot (\nabla h + 1) \tag{11}
\]

Both quantities can easily converted into each other by

\[
j_l = \rho_l \cdot v_l
\]

\[
p_c = \rho_l g \cdot h
\]

\[
K_l = K_h / (100 \cdot 3600 \cdot g)
\]

\[
K_{\text{eff}} = K_{\text{sat}} / (100 \cdot 3600 \cdot g) \tag{12}
\]

\[
K_l(\theta) = K_h(\theta / \theta_{\text{eff}}) \cdot K_{\text{eff}} \tag{13}
\]

Equation (13) in combination with (4) and (12) converts the hydraulic conductivity \( K_h(\theta) \) given in physical units of cm/h to the liquid water conductivity \( K_l(\theta) \) in physical units of s (just a vertical shift in decadal logarithmic scale). Fig 8 displays the resulting liquid water conductivity of Silt.

The derived liquid water conductivity function \( K_l(\theta) \) is used to generate a data set of 101 equidistant value pairs for the range of \( \theta =\{0...\theta_{\text{eff}}; \text{ step } \theta_{\text{eff}}/100\} \), which is exported to the DELPHIN5 / DELPHIN6 material file.
Note, \( D_{\text{v,air}}(T) \) is the diffusion coefficient of water vapour in still air and \( \mu \) is the vapour diffusion resistance factor that accounts for the effects of porosity and tortuosity of the materials. The function \( f(\theta) \) models the effects of blocking of pores by liquid water and diffusion “shortcuts” created by liquid islands. According to [10], the diffusion coefficient of water vapour in free air depends on temperature but the factor \( D_{\text{v,air}}(T)/T \) is almost constant. Consequently the vapour conductivity can be regarded as only-moisture dependent function \( K_v(\theta) \) with two parameters: \( \mu \) and \( f(\theta) \).

For the generation of the moisture dependent water vapour conductivity of soils, we neglect diffusion “shortcuts” created by liquid islands and take the simplest approach \( f(\theta) = (\theta_{\text{eff}} - \theta)/\theta_{\text{eff}} \) that just accounts for blocking of pores. This function is implemented in DELPHIN6 as the “default” case. Then, the only remaining parameter to be determined is the vapour diffusion resistance factor \( \mu \).

Vapour diffusion resistance factors are not measured in soil physics but they are available in building physics. Therefore, we need to estimate them by establishing a relation to a “known” property of the soils, which is the bulk density. Since \( \mu \) accounts for effects of porosity, it can be expected that \( \mu \) will be proportional to the bulk density. This assumption has been checked by using measured material data from Building Physical Research Laboratory of the Institute of Building Climatology at TU Dresden being available in the DELPHIN6 material database. In total, 19 bricks and 45 plasters / mortars were analysed (Fig 9).

The resulting equation (17) in combination with tabulated soil density data given in Table 2 are used to generate the water vapour conductivity of soils. The data set in Table 2 is based on measurements of the classified soils from 15 German locations. Their average values are taken as input to (17), and the received \( \mu_{\text{soil}} \) -values are copied to the material file’s transport base parameters section.
Table 2. Bulk density data of soils according to [3].

<table>
<thead>
<tr>
<th>Reference location</th>
<th>Sand</th>
<th>Loamy Sand</th>
<th>Sandy Loam</th>
<th>Loam</th>
<th>Silt</th>
<th>Silty Loam</th>
<th>Sandy Clay</th>
<th>Loam</th>
<th>Silty Clay</th>
<th>Sandy Clay</th>
<th>Silty Clay</th>
<th>Clay</th>
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</tbody>
</table>

6 Generation and export of the DELPHIN material file

Following the procedure as described in the previous sections of this paper allows generating the first version of a DELPHIN5 / DELPHIN6 material file (Fig 10).

DELPHIN6 material files are ASCII files containing the relevant information divided into sections for identification, base parameters, storage and transport functions. The data sets identified by the keyword FUNCTION are the generated moisture storage function, its reverse function, the liquid water conductivity and the thermal conductivity. A vapour conductivity is not specified since its default approach is used. In simulation projects, DELPHIN6 interpolates the given numerical data of the functions by cubic splines. That brings the advantage that any (valid) model can be used to generate material functions.

The SoilGenerator exports of the data to a material file “soil.m6” automatically once all functions are generated. A user-specific export directory can be selected; otherwise, a subdirectory “materials” is created under the current folder of the SoilGenerator.

7 Determination of the water uptake coefficient

It should be noted that the AW-value, which is the water uptake coefficient \( A_W \), is still unknown (left out in Fig 10). Therefore, a default value of 1 kg/m\(^2\)s is taken in the first place in order to create a valid material file for hygrothermal simulation.
Since a valid liquid water conductivity is given, the determination of the water uptake coefficient is not mandatory. Correct simulation results would be received if the soil is used “as it is”. On the other hand, parameter variations are sometimes of interest. In this case, the water uptake coefficient must be properly determined beforehand.

It can be shown that relation (18) holds as long as the moisture storage function remains unchanged. The factor \( k \) in (18) can be determined by a simulated water uptake (suction) experiment as described in [11] (Fig 11).

\[
K_{eff} = k \frac{A_W}{\theta_{eff}}
\]  

(18)

With a given liquid water conductivity function and a calculated water uptake coefficient from the simulated water mass as function of square root of time, the factor \( k \) is fixed. Then, a parameter variation of \( A_W \) can be converted to a scaling of \( K_l(\theta) \), which is one of the features provided by the DELPHIN5-GUI if both, \( A_W \) and \( K_l(\theta) \), are given in the material file.

![Figure 11. Simulated water uptake (suction) experiment of Silt.](image)

A DELPHIN5 project template is set up in the SoilGenerator in which a material sample of 7 cm height is discretized and a water contact boundary condition is assigned to the bottom surface. The lateral sides are considered adiabatic and moisture tight. The top side is diffusion open.

In the project template, the placeholders of the material reference and the output file name are replaced by the respective soil data, the project file is exported and the DELPHIN5 solver is called to simulate the water uptake process. After that, the SoilGenerator automatically analyses the output file in order to determine the water uptake coefficient of the soil. Finally, the material file is updated with the correct water uptake coefficient and is exported again to the target directory.

8 Conclusions and outlook

The SoilGenerator software implemented on Excel basis allows fast and convenient generation of soil properties according to the DELPHIN5 / DELPHIN6 material file specification. A package “DELPHIN Soil Generator.7z” with the SoilGenerator Version 1.3.2 (in German), the DELPHIN5 solver and three dynamic link libraries (dlls) required by the solver is freely available\(^d\). The interested user should copy and unpack the *.7z file to his own target directory and then execute the Excel file. Some initial settings need to be done on the “ChangeLog” worksheet. The three working steps to be carried out are associated with the buttons on the “VanGuenchten” worksheet.

The output from the SoilGenerator is already being used in research and development projects, for example in Bad Nauheim (Figure 12). The hygrothermal behaviour of the ground is simulated together with the cold district heating network. Fig 13 shows the fields of temperature and ice content at a certain time point during winter time.

![Figure 12: Installation of ground heat collectors in the rural development area of Bad Nauheim South](image)

![Figure 13. Temperature and ice field of the soil calculation domain (20 x 25 m) with one embedded collector field.](image)

In the introduction of this paper, two Joint Research Projects entitled “Soil Ice Storage and Near-surface Geothermics” (ErdEisI and ErdEisII) were mentioned. In ErdEisI, laboratory measurements of soils were conducted in the Building Physical Research Laboratory of the Institute of Building Climatology at TU Dresden in order to derive better knowledge about the hygrothermal properties of soils. For example, one point of criticism could be that the liquid water conductivity is just converted from the van Genuchten parameters. Probably an additional calibration step could be required to receive a better quality of the liquid water conductivity. An experimental validation of this procedure is still part of the current research activities.

A second activity worth to mention is that the dynamic simulation of the ground heat collectors and the cold district heating network in ErdEisII. This requires coupling of different simulation programs, DELPHIN6 for high performance simulation of large problems (the

\(^d\) Download from the TU Dresden cloud service under https://cloudstore.zih.tu-dresden.de/index.php/s/9SH69F6LXHJm589m
ground is discretized up to a width of 100 m and a depth of 20 m) and the AixLib\(^e\) for dynamic simulation of district networks. Both programs must support the Functional Mock-up Interface (FMI) standard\(^f\), which is a tool independent standard to support both model exchange and co-simulation of dynamic models using a combination of xml-files and compiled C-code. In addition, the development of a simulation master\(^g\) was necessary, which is an outcome of the EnTool:CoSim project\(^h\).

The development of the SoilGenerator will be continued to adapt better to the practical engineering processes. For example, geological surveys usually report the stratification of the soil density and the silt, sand and clay percentages in different horizons. The automatic conversion of a geological survey into a DELPHIN6 project with validated soil properties is the final target of the SoilGenerator development.

References


\(^e\) AixLib is a Modelica model library for creating building and system simulations. The library is being developed at the E.ON Energy Research Center, Chair for Building and Indoor Climate Technology at RWTH Aachen University. Download link: http://ibpsa-germany.org/wordpress/tools

\(^f\) Homepage of the FMI standard: https://fmi-standard.org

\(^g\) MASTERSIM is a free tool to coordinate co-simulation Download link: http://ibpsa-germany.org/wordpress/tools

\(^h\) EnTool:CoSim was a collaborative research project (01.01.2014 - 31.12.2017) financially funded by the German Federal Ministry for Economic Affairs and Energy under file number BMWi 02E23S6205