Pedotransfer functions for hydraulic and thermal properties of soil and the tool HERCULES

J. Stolte
J.G. Wesseling
J.H.M. Wösten

Report 126

- 7 JAN. 1997

DLO Winand Staring Centre, Wageningen (The Netherlands), 1996
ABSTRACT


Scientists have developed complex computer models to simulate water and solute movement in the unsaturated and saturated zones. Lack of relevant input data is considered a major obstacle to progress. Therefore, existing databases have been used to derive input data from measured soil data. Pedotransfer functions (PTFs) have been selected for predicting hydraulic and thermal properties using soil texture data. We still lack data from peat and coarse sandy soils for the production of PTFs. The PTFs have been programmed in the computer model HERCULES in order to ease the use of the functions.

Keywords: computer simulation, soil data, soil physics

ISSN 0927-4537

©1996 DLO Winand Staring Centre for Integrated Land, Soil and Water Research (SC-DLO)
P.O. Box 125, NL-6700 AC Wageningen (The Netherlands)
Phone: 31 (317) 474200; fax: 31 (317) 424812; e-mail: postkamer@sc.dlo.nl

No part of this publication may be reproduced or published in any form or by any means, or stored in a database or retrieval system, without the written permission of the DLO Winand Staring Centre.

The DLO Winand Staring Centre assumes no liability for any losses resulting from the use of this report.

Project 579

[Rep126.HM/10.96]
## Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preface</td>
<td>7</td>
</tr>
<tr>
<td>Summary</td>
<td>9</td>
</tr>
<tr>
<td>1 Introduction</td>
<td>11</td>
</tr>
<tr>
<td>2 Soil hydraulic characteristics</td>
<td>13</td>
</tr>
<tr>
<td>2.1 Introduction</td>
<td>13</td>
</tr>
<tr>
<td>2.2 Indirect methods for predicting hydraulic characteristics</td>
<td>14</td>
</tr>
<tr>
<td>2.3 Continuous pedotransfer functions</td>
<td>15</td>
</tr>
<tr>
<td>2.4 Discussion</td>
<td>18</td>
</tr>
<tr>
<td>3 Soil thermal characteristics</td>
<td>21</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>21</td>
</tr>
<tr>
<td>3.2 Thermal transfer functions</td>
<td>22</td>
</tr>
<tr>
<td>3.2.1 Thermal capacity</td>
<td>22</td>
</tr>
<tr>
<td>3.2.2 Thermal conductivity</td>
<td>23</td>
</tr>
<tr>
<td>3.3 Discussion</td>
<td>24</td>
</tr>
<tr>
<td>4 Discussion and conclusions</td>
<td>25</td>
</tr>
<tr>
<td>5 The HERCULES computer model</td>
<td>27</td>
</tr>
<tr>
<td>5.1 Functional description</td>
<td>27</td>
</tr>
<tr>
<td>5.2 System requirements</td>
<td>27</td>
</tr>
<tr>
<td>5.3 Installation</td>
<td>27</td>
</tr>
<tr>
<td>5.4 Using the program</td>
<td>28</td>
</tr>
<tr>
<td>5.4.1 Introduction</td>
<td>28</td>
</tr>
<tr>
<td>5.4.2 The different pages</td>
<td>28</td>
</tr>
<tr>
<td>5.5 Example</td>
<td>30</td>
</tr>
<tr>
<td>5.6 Inside the program</td>
<td>32</td>
</tr>
<tr>
<td>5.6.1 Introduction</td>
<td>32</td>
</tr>
<tr>
<td>5.6.2 Design</td>
<td>32</td>
</tr>
<tr>
<td>5.6.3 Objects</td>
<td>33</td>
</tr>
<tr>
<td>References</td>
<td>37</td>
</tr>
</tbody>
</table>
Preface

The presented study is carried out within program 207 'Development and improvement of instruments for environmental policy analysis' of the DLO Winand Staring Centre. The study started in autumn 1995 and finished in summer 1996.

Report 126 is a first contribution to meet the lack of input data for models on soil hydraulic and thermal properties. As the reader will notice, the procedure is not complete. Assumptions are made for certain situations of the thermal conductivity and not all soil types are covered. Remarks from users of the HERCULES computer program will be appreciated by the authors so that it meets the objectives.

Though pedotransfer functions are good tools to predict soil properties, they are as good as the original measured data from which they were derived. That means that measurement efforts still remain necessary to improve pedotransfer functions.
Summary

Intensive agricultural and industrial activities in many regions cause the quality of our soils and waters to deteriorate. In order to partly control and ultimately rectify this damage, scientists have developed complex computer models to simulate water and solute movement in the unsaturated and saturated zone of the earth’s crust. Nowadays, in various fields of model application such as hydrology, environmental pollution, or global climate change, the lack of relevant characteristics is considered to be a major obstacle to progress. Therefore, it is beneficial to analyse existing data bases in a way that allows input data to be predicted from existing measured soil data if their direct measurement is difficult.

Examples of these pedotransfer functions are used to predict hydraulic and thermal properties of soil from texture data. For the hydraulic properties, the water retention and hydraulic conductivity characteristics are concerned and for the thermal properties the heat capacity and thermal conductivity. The pedotransfer functions for the hydraulic properties are based on predictions of the Mualem-Van Genuchten equations parameters using regression analysis. The heat capacity transfer function is based on the heat capacity of the individual soil particles, and the thermal conductivity transfer function is based on a physical relation, presented by De Vries (1966).

Pedotransfer functions are only as good as the original measured data from which they were derived. This suggests that pedotransfer functions should be periodically updated as more measured data become available. The here presented pedotransfer functions for the soil hydraulic properties only deal with mineral soils with a median particle size < 210 μm (and because the thermal properties depend on the hydraulic functions, this also counts for these properties). For peat soils, a pedotransfer function has still to be distinguished from measured data. Until now, not enough data are available to create such a pedotransfer function.

The pedotransfer functions are programmed in the computer model HERCULES in order to ease the use of the functions. The program requires texture data only. The hydraulic and thermal properties are then calculated and can be printed to file directly.
1 Introduction

Intensive agricultural and industrial activities in many regions cause the quality of our soils and waters to deteriorate. The use of fertilizers, pesticides, and inorganic and organic chemicals has already caused considerable environmental damage (Eijsackers and Hamers, 1993).

In order to partly control and ultimately rectify this damage, scientists have developed complex computer models to simulate water and solute movement in the unsaturated and saturated zone of the earth’s crust. These models have now become indispensable in research directed towards quantifying and integrating the most important physical, chemical and biological processes taking place in these zones of agricultural soils (Addiscott and Wagenet, 1985). Models ranging from very simple to highly complex are being used in a wide variety of studies, such as land evaluation, water management, soil protection, predictive studies, and global climate change (e.g., Boesten and Van der Linden, 1991; Kabat et al., 1992; Teng and Penning De Vries, 1992).

Because environmental changes are not restricted by country borders, there is a general consensus that they should be studied in a global context. As a consequence, international organizations in the field of agriculture and environment are funding projects which can contribute to the development of more sustainable use of our soils and waters. The use of models for research and management has shown that many input data have to be quantified in order to make reliable predictions. At the same time these data are usually fragmented, of different degree of detail, of varying reliability, and are held in different institutes scattered over the world. It is therefore important to develop methods that overcome these limitations.

Nowadays, in various fields of model application such as hydrology, environmental pollution, or global climate change, the lack of relevant characteristics is considered to be a major obstacle to progress. It is recognized that as our ability to numerically simulate complicated flow and transport systems increases, reliability of model predictions may well depend on the degree of detail with which we can estimate model input data such as climate, rooting patterns, water-table fluctuations, soil chemical characteristics, soil hydraulic characteristics (Van Genuchten and Leij, 1992), and soil thermal characteristics. The latter characteristics (thermal conductivity, heat capacity, water retention and hydraulic conductivity) are key characteristics in this respect. The problem is also aggravated by the awareness of the significance of effects of temporal and spatial variability in hydraulic and thermal characteristics on model results, which means that many more samples are needed than previously thought to properly characterize a given field (Warrick and Myers, 1987). Besides variation in hydraulic and thermal characteristics from one location to the other, there is also an important temporal variability in these soil properties. For example, cultivation practices, shrink- and swell- phenomena, and soil crusting cause hydraulic and thermal characteristics to vary with time (e.g. Stolte et al., 1996).
Input data required for simulations can be obtained from direct measurements using different laboratory and field techniques (e.g., Klute, 1986; Page et al., 1982). However, the problem is that the majority of these techniques are relatively time-consuming and costly. At the same time, good predictions instead of direct measurements of input data may be accurate enough for many applications. Therefore, the need to make new measurements has to be critically evaluated considering both the desired accuracy of the input data and the available financial resources to measure them. It is necessary to evaluate whether a balance in levels of detail of the different input data exists as well as in the level of detail of the applied simulation model.

Therefore, it is beneficial to analyse existing data bases in a way that allows input data to be predicted from existing measured soil data if their direct measurement is difficult. An example is the prediction of soil hydraulic characteristics from data recorded in soil surveys, such as clay, silt, and organic matter content percentages. This latter procedure is called an indirect method or pedotransfer function (PTF) approach (e.g., Bouma and Van Lanen, 1987; Larson and Pierce, 1991; Hamblin, 1991). Larson and Pierce (1991) present a limited list of available PTF’s and discuss their role in providing a minimum set of soil data required to assess soil quality. Another way of predicting properties of soil using relatively simple to obtain data is to develop more or less physical based concepts and calibrate parameters on an existing data set. An example of this PTF approach is the De Vries equation for the thermal conductivity (De Vries, 1966).

To facilitate general use of the developed PTF’s, this report gives a description of the computer program HERCULES. This program uses existing PTF’s to predict in an user-friendly way the water retention, hydraulic conductivity, thermal conductivity, and heat capacity characteristics of mineral soils. In the second chapter of this report the theory of the PTF’s for the hydraulic characteristics that are used in HERCULES is described. The third chapter deals with the theory of the PTF’s for the thermal characteristics. This is followed by a discussion about these two approaches in the fourth chapter. The fifth chapter finally presents the computer program HERCULES and provides a manual on how to work with the model.
2 Soil hydraulic characteristics

2.1 Introduction

Darcy’s law states that water flux in porous media equals hydraulic conductivity times gradient of soil water potential. Combination of Darcy’s law with the expression for conservation of mass, yields the Richards (1931) partial differential equation for soil moisture flow in unsaturated soil:

\[
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} - 1 \right) \right] \tag{1}
\]

where \( h \) is the soil water pressure head (cm), \( \theta \) is the volumetric water content (-), \( K \) is the hydraulic conductivity (cm/d), \( t \) is time (d), and \( z \) is soil depth (cm). In order to solve this equation, information is needed on the \( h(\theta) \) water retention- and \( K(\theta) \) or \( K(h) \) conductivity relationships. Because of their importance much work has been done in order to establish accurate values for these relationships. Roughly speaking, investigations to determine the relationships can be divided into a direct measurement approach and an indirect prediction approach.

Smith and Mullins (1991) gave an overview of laboratory and field techniques for direct measurement of the soil hydraulic characteristics. Many direct measurement techniques require steady-state conditions and are based on direct approximations of Darcy’s law. Many transient methods are also widely used, such as the hot-air, sorptivity, disc permeameter, and instantaneous profile method. Although these methods are relatively simple in concept, they have the disadvantage that they are often time consuming (waiting for steady state), and that a number of boundary conditions must be obeyed.

A variation on direct measurement techniques is the inverse modelling approach in which a flow experiment in the laboratory is simulated by estimating the hydraulic characteristics in such a way that differences between properties, such as observed and calculated water contents, pressure heads and/or flow rates, are minimized (Dane and Hruska, 1983; Kool et al., 1987). In this approach, additional information is often required to ensure uniqueness of the predicted characteristics. Feddes et al. (1993) demonstrated that inverse modelling is also applicable on large scales when remote sensing is used to determine areal evaporation and surface moisture. Care should be taken in the latter approach that not all of the uncertainty is lumped in the determination of the soil hydraulic characteristics.

Developments in electronic and computer technologies will probably improve measurement procedures and result in computer-driven, stand-alone devices. Despite these efforts, the fact remains that at the present time direct measurement of hydraulic characteristics is notoriously difficult and costly, especially for undisturbed field soils (Van Genuchten and Leij, 1992).
2.2 Indirect methods for predicting hydraulic characteristics

Whereas much attention has been paid to the development of direct methods for measurement of hydraulic characteristics, relatively little attention has been paid to the development of indirect methods to predict hydraulic characteristics from more easily measured data. The latter type of data might be routinely recorded in soil surveys for example clay, loam and organic matter percentages or data on particle-size distribution or water retention. These indirect methods have a clear advantage over direct methods because they are far less costly and are generally more convenient to use. A possible disadvantage is that indirect methods offer a prediction and not a measurement of the hydraulic characteristics.

In numerous cases practical applications do not require very accurate hydraulic characteristics, and therefore predictions made with these indirect methods may be sufficient. When using indirect methods two different approaches can be used. In the first approach, the more difficult to measure characteristic, hydraulic conductivity, is predicted from the more easily measured characteristic, water retention. In the second approach, hydraulic characteristics are predicted from data recorded in soil surveys where no measured hydraulic characteristics are involved. It is important to note that no indirect methods exist without direct methods to measure the hydraulic characteristics. Only direct measurements will create a data base from which indirect methods can be derived to predict hydraulic characteristics. Therefore, development of indirect methods does not imply that continued research towards improved direct methods is obsolete.

A good state-of-the-art of the indirect methods and available pedotransfer functions is given by Wösten (1996) where a distinction is made between class and continuous PTF’s. Continuous pedotransfer functions that predict specific points of interest on the $\theta - h - K$ relationships have been developed by several researchers (Gupta and Larson, 1979; Poelman and Van Egmond, 1979; Rawls et al., 1982; Ahuja et al., 1985). These functions often have the following form:

$$\text{water content } \theta \text{ (at, for example, } h = -100 \text{ cm)} = b_0 + b_1*C + b_2*OM + b_3*D + ... + b_x*X.$$  

In this equation $C$ is percent clay, $OM$ is percent organic matter, $D$ is bulk density, and $X$ any other basic soil property that can easily be determined. Parameters $b_0$ through $b_x$ are determined by regression of $\theta$ at for example $h = -100$ cm versus relevant soil properties. A disadvantage of using continuous pedotransfer functions for predictions of specific points of interest is that a large number of different functions are required to describe the complete $\theta - h - K$ relationship. This feature strongly hampers the efficient inclusion of hydraulic characteristics in simulation models. Alternatively, parameterization methods are used that predict parameters in a model describing the $\theta - h - K$ relationship. This latter approach is more efficient than the point-prediction procedure. An example of this procedure is presented by Wösten et al. (1995). The computer program HERCULES, described in this report, uses PTF’s presented by Wösten (1996) to predict the water retention and hydraulic conductivity characteristics for mineral soils.
2.3 Continuous pedotransfer functions

Over the years and in a number of different research projects, soil water retention and hydraulic conductivity curves have been measured for a large number of soils in the Netherlands. As a set, the curves form a unique data base covering a broad spectrum of soils. Hydraulic conductivities are measured using a combination of the following five methods:

(i) The column method for vertical saturated hydraulic conductivity, $K_s$.

(ii) The crust-test for unsaturated conductivities when the pressure head, $h$, is between 0 and -50 cm.

(iii) The sorptivity method for conductivities of coarse-textured soils when $h \leq -50$ cm.

(iv) The hot-air method for conductivities of medium- and fine-textured soils when $h \leq -50$ cm.

(v) The evaporation method for hydraulic conductivities when $h$ is between 0 and -800 cm.

Soil water retention curves are obtained by slow evaporation of wet, undisturbed samples in the laboratory. Pressure heads are measured periodically with transducer-tensiometers and subsamples are taken at the same time to determine water contents. Alternatively, water contents are also determined by weighing the total sample at each pressure head. Both methods yield points relating $h$ to the water content $\theta$.

Water contents corresponding to pressure heads lower than -800 cm are obtained by conventional methods using air pressure. Details on the applied measurement techniques are given by Stolte et al. (1992) and by Wopereis et al. (1994). The effort to measure hydraulic characteristics for a variety of soils resulted in a data base comprising 620 measured characteristics (Wosten et al., 1994).

To derive continuous pedotransfer functions for soils in the Netherlands, all individually measured hydraulic characteristics were parameterized using the equations of Van Genuchten (1980).

\[
\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^{1/n}}
\]  

\[
K(h) = K_s \left(\frac{(1 + |\alpha h|^n)^{1/n} - |\alpha h|^n}{(1 + |\alpha h|^n)^{(1+n)/(1+2)}}\right)^2
\]

In these equations the subscripts $r$ and $s$ refer to residual and saturated values and $\alpha$, $n$ and $l$ are parameters that determine the shape of the curve. The residual water content $\theta_r$ refers to the water content where the gradient $d\theta/dh$ becomes zero ($h \to -\infty$). In practice $\theta_r$ is the water content at some large negative value of soil-water pressure head. The parameter $\alpha$ (cm$^{-1}$) approximately equals the inverse of the pressure head at the inflection point where $d\theta/dh$ has its maximum value. The dimensionless parameter $n$ determines the rate at which the S-shaped retention curve turns towards the ordinate for large negative values of $h$, thus reflecting the steepness of the curve.
The dimensionless parameter \( l \) determines the slope of the hydraulic conductivity curve in the range of more negative values of \( h \). Although \( l \) is presumably a soil specific parameter, Mualem (1976) concluded from an analysis of 45 soil hydraulic data sets that \( l \) should be, on average, about 0.5. In this study \( l \) is not fixed but is considered to be one of the experimental unknowns. As follows from the equations, the parameter \( \theta \), affects only the shape of the retention curve while leaving the conductivity function unaffected. The parameter \( l \), on the other hand, affects the hydraulic conductivity only and leaves the retention curve unchanged. The flexibility of the equations in generating different shapes of \( \theta(h) \) and \( K(h) \) relationships has been demonstrated by a number of researchers (e.g., Hopmans and Overmars, 1986; Wösten and Van Genuchten, 1988).

The nonlinear least-squares optimization program RETC (Van Genuchten et al., 1991) is used to predict the unknown parameters (\( \theta_r \), \( \theta_s \), \( K_r \), \( \alpha \), \( l \) and \( n \)) in both equations simultaneously from measured soil-water retention and hydraulic conductivity data. In the optimization procedure the sums of squares of differences between measured and predicted water contents and between measured and predicted hydraulic conductivities are minimized.

After parameterization, linear regression was used to investigate the dependency of each model parameter on more easily measured basic soil properties. To comply with a number of physical boundary conditions, transformed parameters rather than the original model parameters are used in the regression analysis. In the case of sandy soils the imposed boundary conditions are: \( K_s > 0 \), \( \alpha > 0 \), \( n > 1 \), and \(-2 < l < +2\). In the case of loamy and clayey soils the latter boundary condition is \(-10 < l < +10\). As a consequence, parameters are transformed as follows: \( K'_r = \ln(K_r) \), \( \alpha' = \ln(\alpha) \), \( n' = \ln(n-1) \); for sandy soils \( l' = \ln((l+2)/(2-l)) \), and for loamy and clayey soils, \( l' = \ln((l+10)/(10-l)) \). For sandy soils the following basic soil properties are used as regressed variables: percent clay + silt; percent organic matter; bulk density; median sand particle size; and also the qualitative variable topsoil or subsoil. For loamy and clayey soils, the regressed variable percent clay + silt is replaced by percent clay.

Linear, reciprocal, and exponential relationships of these basic soil properties are used in the regression analysis, and possible interactions are also investigated. As a consequence, the resulting regression model or continuous PTF consists of various basic soil properties and their interactions, all of which contribute significantly to the description of the transformed model parameters. This model is selected with the subset selection method of Furnival and Wilson (1974). The resulting continuous PTF's are presented in Table 1. After prediction of the transformed model parameters with these functions, the hydraulic characteristics are obtained by back-transformation to the original model parameters (Wösten et al., 1995).
Table 1. Continuous pedotransfer functions for the prediction of hydraulic characteristics and bulk density of mineral soils in the Netherlands (after Wosten, 1996)

<table>
<thead>
<tr>
<th>Continuous PTF's for sandy soils:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_s$</td>
<td>$- 13.6 - 0.0153^*CS + 0.0000836^*CS^2 - 0.0973^*CS^{-1} + 0.708^*D^{-1} - 0.00703^*M50^+225.3^<em>M50^{-1} + 2.614^</em>\ln(M50) + 0.0084^<em>OM^{-1} + 0.02256^</em>\ln(OM) + 0.00718^*D^*CS \quad (R^2 = 71%)$</td>
</tr>
<tr>
<td>$K_s^*$</td>
<td>$9.5 - 1.471^*D^2 - 0.688^*OM + 0.0369^<em>OM^2 - 0.332^</em>\ln(CS)$ \quad (R^2 = 32%)</td>
</tr>
<tr>
<td>$\alpha^*$</td>
<td>$146.9 - 0.0832^*OM - 0.395^*topsoil - 102.1^*D + 22.61^*D^2 - 70.6^*D^{-1} - 1.872^<em>CS^{-1} - 0.3931^</em>\ln(CS)$ \quad (R^2 = 53%)</td>
</tr>
<tr>
<td>$n^*$</td>
<td>$0.797 - 0.591^*OM + 0.0677^*OM^2 + 0.573^*topsoil$ \quad (R^2 = 42%)</td>
</tr>
<tr>
<td>$1/D$</td>
<td>$- 1.984 + 0.01841^*OM + 0.032^*topsoil + 0.00003576^*CS^2 + 67.5^<em>M50^{-1} + 0.424^</em>\ln(M50)$ \quad (R^2 = 72%)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Continuous PTF's for loamy and clayey soils:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_s$</td>
<td>$0.8085 - 0.2617^*D - 0.038^*topsoil + 0.00001046^<em>C^2 + 0.01287^</em>\ln(OM)+0.000789^*C^*topsoil \quad (R^2 = 86%)$</td>
</tr>
<tr>
<td>$K_s^*$</td>
<td>$- 43.1 + 64.8^*D - 22.21^*D^2 + 7.02^*OM - 0.1562^<em>OM^2 + 0.985^</em>\ln(OM)-0.01332^*C^*OM - 4.71^*D^*OM \quad (R^2 = 30%)$</td>
</tr>
<tr>
<td>$\alpha^*$</td>
<td>$11 - 2.298^*D^2 - 12.41^*D^{-1} + 0.838^*OM + 0.343^<em>OM^{-1} + 2.03^</em>\ln(OM)\quad 1.263^*D^*OM \quad (R^2 = 51%)$</td>
</tr>
<tr>
<td>$l^*$</td>
<td>$0.451 + 2.678^<em>D^{-1} - 1.093^</em>\ln(C)$ \quad (R^2 = 44%)</td>
</tr>
<tr>
<td>$n^*$</td>
<td>$- 0.34 + 1.224^<em>D^{-1} - 0.7952^</em>\ln(C) - 0.3201^*\ln(OM) + 0.0651^*D^*OM \quad (R^2 = 74%)$</td>
</tr>
<tr>
<td>$1/D$</td>
<td>$0.603 + 0.003975^*C + 0.00207^<em>OM^2 + 0.01781^</em>\ln(OM) \quad (R^2 = 77%)$</td>
</tr>
</tbody>
</table>

$\theta_s, K_s^*, \alpha^*, l^*, \text{and } n^*$ are the transformed model parameters in the Van Genuchten - Mualem equations; $C$ is percent clay (i.e. percent < 2 μm); $CS$ is percent clay + silt (i.e. percent < 50 μm); $OM$ is percent organic matter; $D$ is bulk density; $M50$ is median sand particle size; $\text{topsoil}$ and $\text{subsoil}$ are qualitative variables having the value of 1 or 0 and $\ln$ is the natural logarithm.

A comparable approach to derive continuous PTF's for different soils has been employed by a number of researchers (e.g., Ghosh, 1980; Cosby et al., 1984; Rawls and Brakensiek, 1985; Saxton et al., 1986; Gregson et al., 1987; Vereecken et al., 1989, 1990). Tietje and Tapkenhinrichs (1993) compared 13 different PTF's with respect to their applicability and accuracy in predicting measured water retention functions. The evaluated PTF's consisted of point-prediction methods and model parameter prediction methods for the prediction of the water-retention function. They concluded that the latter method using the empirical equation of Van Genuchten (1980) was the most practical and the most accurate approach. It was emphasized that prediction procedures performed poorly if used for soils that fall outside the texture range of soils originally used to derive the PTF's. Therefore, the use of PTF's to predict hydraulic characteristics should be confined to soils with a texture within the range of textures of soils that were originally used to derive the PTF's.
The same set of Dutch soils as used to derive continuous PTF's for the prediction of hydraulic characteristics was used also to derive continuous PTF's for the prediction of the bulk density of the soil (actually the reciprocal value or specific volume in cm$^3$ g$^{-1}$ was predicted). Use of the same statistical techniques resulted in two continuous PTF's, one for sandy soils and one for loamy and clayey soils, that predict the specific volumes of these soils (Table 1).

An attractive feature of continuous PTF's is that the uncertainty involved in using them can be quantified. Wösten and Van Genuchten (1988) expressed the uncertainty involved in using continuous PTF's in terms of 90% confidence intervals. They concluded that because the confidence intervals are relatively wide, predictions made with their PTF's will show considerable dispersion. Alternatively the PTF's can be used to predict model parameters for the same set of soils as from which the PTF's were derived. Differences between 'measured' and 'predicted' model parameters can be expressed in a variance-covariance matrix. In turn, this matrix allows prediction of average hydraulic characteristics of a soil for which no measured characteristics are available, as well as a quantification of uncertainty of the predicted average characteristics. More details on this approach are provided by Vereecken et al. (1992) and Finke et al. (1996). The latter researchers used the PTF's not only to predict the mean hydraulic characteristics of a soil but also to predict 20 hydraulic characteristics expressing the uncertainty in the applied PTF. In turn, they used the 20 hydraulic characteristics in a Monte Carlo procedure to calculate a number of different aspects of functional soil behaviour. Their approach showed to what extent variability in calculated aspects of soil behaviour is explained by uncertainty in PTF's.

2.4 Discussion

Continuous PTF's are regression models that use various basic soil properties and their interactions as regressed variables. Complications might occur in the selection of which basic soil properties are to be used as regressed variables. This is best illustrated by an example where the PTF has two regressed variables: $X_1$ and $X_2$. In this case three situations are possible (Oude Voshaar, 1994):

(i) The part of the sum of squares accounted for by $X_1$ and $X_2$ in a combined regression model equals the sum of the sum of squares accounted for by $X_1$ and $X_2$ in separate regression models. In this case the regression coefficients in the combined model equal those in the separate models.

(ii) The part of the sum of squares accounted for by $X_1$ and $X_2$ in a combined regression model approximately equals the sum of squares accounted for by $X_1$ and $X_2$ in the separate regression models.

(iii) The part of the sum of squares accounted for by $X_1$ and $X_2$ in a combined regression model is much larger then the sum of the sum of squares accounted for by $X_1$ and $X_2$ in the separate models.

In situation (i) the regressed variables $X_1$ and $X_2$ are said to be orthogonal. In situation (ii) one regressed variable can be replaced by the other. An example of the latter case is pH determined in water and pH determined in KCl. In this situation when the
regressed variables are strongly correlated, the problem of multicollinearity is said to exist (Montgomery and Peck, 1982). In situation (iii) the regressed variables $X_1$ and $X_2$ supplement each other.

Consequences are that in a balanced sampling strategy (situation (i)) variables, such as the parameters in the Van Genuchten equations, are predicted correctly and that an explanation can be given as to which of the regressed variables has a strong impact on prediction of the model parameter. In this sense the causality is maintained and the interpretation of the effects is unique, however all these features are lost in the (ii) and (iii).

Inspection of the correlation matrix of regressed variables is a quick and easy way to determine whether some of the variables are strongly linear dependent. In the latter case it is preferred to replace one variable by the other. Multicollinearity often occurs in unbalanced sample strategies as applied in observational research where data are taken as they come. However, many interpretation problems can be avoided by aiming at balanced sampling of regressed variables.

The here presented pedotransfer functions only deal with mineral soil with a median particle size < 210 µm, because of the lack of measurements of organic and coarse soils.
3 Soil thermal characteristics

3.1 Introduction

The temperature at a certain depth in a soil profile is predicted using the partial differential equation for thermal conductivity

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( \frac{\lambda}{\rho c} \frac{\partial T}{\partial z} \right)$$

(4)

where $T$ is soil temperature (°C); $\lambda$ thermal conductivity (W m$^{-1}$ K$^{-1}$); $\rho c$ is volumetric thermal capacity (J m$^{-3}$ K$^{-1}$) (with $\rho$ is wet bulk density and $c$ is specific thermal capacity); $t$ is time (s) and $z$ is depth (m). Both $\lambda$ and $\rho c$ are depended on the texture, water content and temperature of the soil. The latter influence is small compared to the other factors and is usually neglected. Solution of Equation (4) needs information of the $\lambda(\theta)$ thermal conductivity and $\rho c(\theta)$ thermal capacity characteristics. These thermal characteristics can be determined by direct measurements or an indirect prediction, using physically-based equations.

The thermal conductivity can be measured directly using the so-called needle method. A heat probe containing an electrical heater and thermocouple is commonly used for this purpose (e.g., Stålhane and Pyk, 1931; De Vries, 1952; Feddes, 1971; Shiozawa and Campbell, 1990; Campbell et al., 1994). The method is based on a solution of the general thermal conductivity equation for a constant line heat source applied in a homogeneous isotropic medium of initially uniform temperature. Van Haneghem (1981) introduced a calculation procedure that determines the thermal capacity, using the same measurement method.

Direct measurements of the thermal capacity and conductivity are time consuming, especially when the variability of these properties have to be known. The thermal properties can also be derived using indirect methods. A transfer function can be established which predicts $\lambda$ based on texture and water content of the soil. Farouki, 1986 gives a state-of-the-art of the available transfer functions. Several methods are compared. From Farouki it can be concluded that the methods of Johansen, 1975 and De Vries, 1966 give the best predictions of the thermal conductivity. A comparison between these two methods is given in Table 2, where measured and computed results are shown for a sandy soil as presented by De Vries, 1966.
From Table 2 it can be concluded that for relatively wet soils both the Johansen and the De Vries transfer function give accurate predictions of the thermal conductivity. This is also concluded by Farouki (1986), who even found that for the wet part Johansen describes the thermal conductivity more accurately. For the total range from dry to wet, the De Vries results are within 10% of the experimental values, whereas the Johansen results differ up to more than 500%. This justifies the choice to use the De Vries equation to predict the thermal conductivity of a soil.

### 3.2 Thermal transfer functions

#### 3.2.1 Thermal capacity

The thermal capacity of a soil can be calculated using:

\[
\rho c = x_s \rho_s c_s + x_w \rho_w c_w + x_a \rho_a c_a
\]

where \(\rho_s\), \(\rho_w\), and \(\rho_a\) are bulk densities of solid material, water, and air respectively; \(c_s\), \(c_w\), and \(c_a\) are the specific heat per unit solid material, water, and air respectively; and \(x_s\), \(x_w\), and \(x_a\) are the volume fractions solid material, water, and air respectively. Feddes (1971), among others, showed that the capacity per unit \((\rho c)\) of the mineral compounds is \(\rho_{sm} c_{sm} = 1.92 \times 10^6 \text{ J m}^{-3} \text{ K}^{-1}\), for the organic part \(\rho_{so} c_{so} = 2.88 \times 10^6 \text{ J m}^{-3} \text{ K}^{-1}\), and for water \(\rho_{w}c_w = 4.18 \times 10^6 \text{ J m}^{-3} \text{ K}^{-1}\). Since \(\rho_a c_a\) is about 1255 J m\(^{-3}\) K\(^{-1}\) it can be ignored. This results in:

\[
\rho c = (1.92x_{sm} + 2.88x_{so} + 4.18x_w) \times 10^6
\]

where \(x_{sm} + x_{so} + x_w + x_a = 1\).
3.2.2 Thermal conductivity

The thermal conductivity of a soil depends on the water content and texture and can be predicted using the De Vries transfer function. De Vries calculates the thermal conductivity for ellipse-shaped soil parts in a medium of water or air through:

$$\lambda = \frac{x_f \lambda_f + F x_s \lambda_s}{x_f + F x_s}$$  \hspace{1cm} (7)

where \(f\) and \(s\) represent the fluid (or air) and solid phase and \(x\) is the volume fraction. The factor \(F\) is described through:

$$F = \frac{1}{3} \sum_{a,b,c} \left[ 1 + \left( \frac{\lambda_a}{\lambda_f} - 1 \right) g_a \right]^{-1}$$  \hspace{1cm} (8)

where \(g_a + g_b + g_c = 1\). These parameters are the so-called shape factors of the soil particles. For particles with a ellipsoidal shape \(g_a = g_b\) is valid. Because \(g_a = g_b = g_c = \frac{1}{3}\) is also valid, \(g_a\) remains the shape factor to determine. Equation (7) calculates for dry soils \((x/x_f \sim 100)\) a thermal conductivity that is about 25% too low. In these cases, Equation (7) has to be multiplied with 1.25 (De Vries, 1966).

Equation (7) is only valid for situations of ellipsoidal shaped soil particles in a continuous medium of air or water. In the case the pores are partly filled with water and air, Equation (9) has to be used

$$\lambda = \frac{x_f \lambda_f + F_a x_a \lambda_a + F_s x_s \lambda_s}{x_f + F_a x_a + F_s x_s}$$  \hspace{1cm} (9)

where:

$$F_a = \frac{1}{3} \left[ \frac{2}{1 + \left( \frac{\lambda_a}{\lambda_f} - 1 \right) g_{as} \lambda_a^{-1}} + \frac{1}{1 + \left( \frac{\lambda_s}{\lambda_f} - 1 \right) (1-2g_{as})} \right]$$  \hspace{1cm} (10)

and

$$F_s = \frac{1}{3} \left[ \frac{2}{1 + \left( \frac{\lambda_s}{\lambda_f} - 1 \right) g_{as} \lambda_s^{-1}} + \frac{1}{1 + \left( \frac{\lambda_a}{\lambda_f} - 1 \right) (1-2g_{as})} \right]$$  \hspace{1cm} (11)

In the range \(x_{wc} \leq x_f \leq n\), where \(x_{wc}\) is critical water content (here defined as water content at pH 4.2) and \(n\) is porosity, \(g_{as}\) becomes:

$$g_{as} = 0.333 - \left( \frac{x_f}{n} \right) (0.333 - 0.035)$$  \hspace{1cm} (12)
At $x_f < x_{wc}$ De Vries assumes that the air-filled pores are not saturated with water vapour anymore. In this situation the thermal conductivity of air varies linearly with the water content through:

$$\lambda_{air} + \lambda_v = \lambda_a + \left( \frac{x_{wc}}{x_f} \right) (\lambda_v - \lambda_a) \quad (13)$$

The shape factor becomes in this situation:

$$g_{aa} = 0.013 + \left( \frac{x_f}{x_{wc}} \right) (0.098 - 0.013) \quad (14)$$

assuming that the $g_a$ for particles is 0.144.

It is recommended by De Vries to discontinue the calculations with water as a continuous medium at a $x_{wc}$-value of about 0.03 for coarse textured soils and at a $x_{wc}$-value of about 0.05 to 0.10 for fine textured soils. The relation between $\lambda$ and $x_w$ for moisture contents below this value up to $x_w = 0$ can be obtained by interpolation, since the value of $\lambda$ for dry soil can be found using Equation (7).

### 3.3 Discussion

The thermal capacity estimate is a physically-based equation and depends on the values for $\rho_c$ for the various soil compounds. Feddes (1971) stated that the results are within 5 to 10% from the measured value, based on results presented by De Vries (1966).

The De Vries transfer function estimates the thermal conductivity using an empirical model. The accuracy of this estimate is in most cases better than 10% (De Vries, 1966), and can even be improved when the water retention characteristic of the soil is known. The uncertainty of the method is the value of the shape factors. De Vries found for a quartz sand the value 0.144 and for clay 0.125, using diffusion experiments. Also, Feddes (1971) concluded that the shape factor has to be derived from diffusion experiments. Campbell et al. (1994) used the shape factor as fitting parameter, resulting for various soil types in $g_a$ varying from 0.071 (loess) to 0.330 (peat). This indicates that the reliability of the presented equation strongly depends on the estimate of the shape factor. For a first estimate, 0.125 for $g_a$ can be adopted, but it is advisable to measure a set of values representing different soil types. This makes it also necessary to present Equation (14) in terms of the shape factor.
4 Discussion and conclusions

Pedotransfer functions are a powerful tool in estimating physical properties of soils. Because PTF’s predict difficult-to-obtain properties from already available basic soil properties, they have the clear advantage that they are relatively inexpensive and easy to derive and use. Accuracy of PTF’s predictions is sufficient for many applications at regional and national scales since on these scales temporal and spatial variability effects most likely will have a dominant impact on the modelling results. For application at a specific location, use of PTF’s might not be appropriate in which case direct measurement is the only option. PTF’s should not be used to make predictions for soils that are outside the range of soils used to originally derive the PTF’s. In other words, PTF’s may be used safely for interpolation but not for extrapolation. PTF’s are only as good as the original measured data from which they were derived. This suggests that PTF’s should be periodically updated as more measured data become available. To develop useful PTF’s it is important that regressed variables in regression models are not strongly linearly related thus preventing multicollinearity.

The here presented PTF’s for the soil hydraulic properties only deal with mineral soils with a median particle size < 210 μm, (and because the thermal properties are depended on the hydraulic functions, this also counts for these properties). For peat soils, a PTF has still to be distinguished from measured data. Until now, not enough data are available to create such a PTF. In a later version of HERCULES, an estimate will be given for hydraulic properties of peat soils.

Using physically-based equations of the thermal properties of soil is a good way to predict these properties. The function of De Vries leaves an uncertainty in parameterization of the shape factor. This factor has to be established for several soil types, using measurement techniques. It is preferable to derive pedotransfer functions for the thermal properties, in the same way as is done for the hydraulic properties. To fill this gap we need a set of measured thermal conductivities, gathered from a wide range of soil types.
5 The HERCULES computer model

5.1 Functional description

In the first section of this report a description is given of the use of PTF’s for the prediction of hydraulic characteristics. The second part describes the theory of calculating the heat conductivity with the physical-based equation of De Vries and the heat capacity. These two types of functions (hydraulic and thermal) are programmed in the HERCULES computer model. From soil texture data, supplied by the user, it calculates the parameters of the Mualem-Van Genuchten equations which yield the hydraulic conductivity and the water retention characteristics. Combining the latter characteristic with the thermal characteristics of all constituents of the soil, the De Vries’ theory yields the thermal conductivity at the specified moisture content. These data are written into a table presented at screen. The table contains pressure head, hydraulic conductivity, thermal conductivity and thermal capacity for a number of moisture contents. These moisture contents range from θ corresponding to pressure head of $-10^{-9}$ to θ, with an increment of 0.01. An option is available to write the table to a file. Finally the data thus obtained can be seen as graphs.

5.2 System requirements

The program HERCULES has been developed to run on any PC with Windows. There are no hardware requirements, though a VGA of SVGA screen is recommended.

5.3 Installation

The program comes on one diskette containing the following files:
- Hercules.exe
- Hercules.ico
- Hercules.hip

The most simple way to install the program is the following (assuming the user is familiar with Windows):
- Create the directory that should contain the program.
- Copy the files from diskette to the directory on hard disk.
- From the program manager, open or create the group where HERCULES is to be placed.
- With the File I New option, select Program Item.
- Fill in the following fields:
  Description : Hercules
  Command line : Hercules.exe help hercules.hlp
  Working directory : (The directory you created)
Shortcut keys:
- Click on the Change Icon button.
- Click on Browse
- Select <working directory> Hercules.ico
- Click OK twice

Now the program can be started by double-clicking the HERCULES icon.

5.4 Using the program

5.4.1 Introduction

The program HERCULES has been developed to create tables with soil physical data from soil texture data and general thermal data. After starting the program two parts can be seen on screen: the menu bar and the input-output pages. The menu-bar contains two main fields:

File : use this to exit the program
Help : provides on-line help

5.4.2 The different pages

The program has been developed using the so-called tabbed notebook. This means the user can select one page at a time to be visible. The pages can be selected by clicking on one of the tabs on top of the pages or pressing the corresponding key-combination from the keyboard. The pages have names as indicated in Table 3.

Table 3 The different pages of the tabbed notebook and their main purpose

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Texture</td>
<td>Input of all soil texture data</td>
</tr>
<tr>
<td>Van Genuchten</td>
<td>Shows all parameter values of the Mualem-equations and the bulk density</td>
</tr>
<tr>
<td>Elementary data</td>
<td>Input of thermal conductivities and thermal capacities and shape factor</td>
</tr>
<tr>
<td>Table</td>
<td>Shows the calculated table of soil physical data and provides the option to create a data file</td>
</tr>
<tr>
<td>Graphics</td>
<td>Shows graphs of the soil physical data</td>
</tr>
</tbody>
</table>

Some of these pages contain input fields where the user can specify values for his own data. These fields can either be selected by pressing the Tab-key several times or by putting the cursor in the field and clicking the left-hand mouse button. When an attempt is made to leave a field where illegal data was entered, an error message will appear
and control is returned to the same field. You can tell the program to accept the changes by just switching to another page. The different pages will be discussed in more detail.

**Texture**

This page is the first page the user sees after starting the program. It contains the input fields for the soil textural data the program requires. The default values for the fields are taken from Wösten et al. (1995) for an O3-module. The following fields should be filled by the user:

- **Name of soil**: A description of the soil considered
- **Organic matter**: Organic matter content (in %), a value between 0 and 15.
- **Percentage clay**: The percentage of clay (particles < 2 μm), a value between 0 and 100.
- **Percentage silt**: The percentage silt (particles between 2 and 50 μm), a value between 0 and 100.
- **Median particle size of sand**: The median particle size of the sand fraction (particles < 2000 μm) (μm), a value between 0 and 10^5.

The fields with the percentage below 50 μm and the median particle size are only visible when the value in the field for percentage below 2 μm is smaller than 8 (loamy and sandy soils).

At the lower left side of this page a so-called radio-group is placed where it should be indicated whether the data are for a topsoil or a subsoil.

Two buttons can be found at the bottom of the page: Reset and Default. Pressing the Reset-button causes the program to undo the changes you made after entering this page. Pressing Default will reset all fields to the values of the O3-soil. When you enter the page for the first time, these buttons do have the same effect. When you re-enter this page after seeing another page, the effect is different: Reset causes the fields to get the values you just entered before leaving the page, Default assigns the default values. When leaving this page, the data are automatically processed yielding the new parameters of the Mualem-Van Genuchten equations.

**Van Genuchten**

This page does not contain any input fields. It was designed only to show the values of the parameters of the Mualem-Van Genuchten equations and the bulk density calculated with the pedotransfer functions from the data entered in the previous page.

**Elementary data**

This page contains the thermal characteristics of the separate constituents of the soil. The page also contains an input field for the shape-factor of the De Vries' equation (see Chapter 3). This parameter has the default value 0.125. The other default values
are presented in Table 4.

### Table 4

**Default values of parameters used in the De Vries empirical transfer function.**

<table>
<thead>
<tr>
<th>Material</th>
<th>Thermal conductivity (W m(^{-1}) °C(^{-1}))</th>
<th>Thermal capacity (J m(^{-3}) °C(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0.02245</td>
<td>1.26 (10^3)</td>
</tr>
<tr>
<td>Vapor</td>
<td>0.02750</td>
<td>1.26 (10^3)</td>
</tr>
<tr>
<td>Water</td>
<td>0.59080</td>
<td>4.18 (10^6)</td>
</tr>
<tr>
<td>Clay</td>
<td>2.91240</td>
<td>1.92 (10^6)</td>
</tr>
<tr>
<td>Quartz</td>
<td>8.48760</td>
<td>1.92 (10^6)</td>
</tr>
<tr>
<td>Organic material</td>
<td>0.24960</td>
<td>2.88 (10^6)</td>
</tr>
</tbody>
</table>

Just like in the page with textural data, the buttons Reset and Default can be found at the bottom of this page. They have the same meaning.

### Tables

This is the page containing the output table. This table consists of five columns: \(\theta\) (cm\(^3\) cm\(^{-3}\)), \(h\) (cm), \(K\) (cm d\(^{-1}\)), \(\lambda\) (W m\(^{-1}\) °C\(^{-1}\)) and \(C\) (J m\(^{-3}\) °C\(^{-1}\)). These values are presented for a number of moisture contents, starting with the residual moisture content \(\theta_r\), and increasing with a value \(\Delta\) until the value of \(\theta_f\) is reached. This value of \(\Delta\) has been fixed to a value of 0.01 up to now. The table has been presented in a so-called memo. At the right-hand side of the table a scroll-bar is created. Clicking on this scroll bar with the mouse or just pressing the down- or up-arrow in the field of the memo allows the user to make another part of the table visible.

At the bottom of the page a button ‘Write to file’ can be found. Pressing this button calls the default file window where you can indicate to which file the data should be written and in which directory it should be stored.

### Graphs

This page contains 4 graphs: \(h\), \(K\), \(\lambda\) and \(C\), all as a function of \(\theta\).

### 5.5 Example

This section shows the output file generated with the default data.

*The output file*

```plaintext
! File test.out created Friday, 22/3/1996 18:23:03
!
! This file contains data of soil O3
!
!
! Texture data:
```

30
Organic matter percentage: 2.0
Percentage below 2 μm: 1.0
Percentage below 50 μm: 25.0
Median particle size: 160 μm
The soil is a sub soil.

The Van Genuchten parameters:
\[
\theta_r = 0.000 \text{ cm}^3 \text{ cm}^{-3}
\]
\[
\theta_s = 0.371 \text{ cm}^3 \text{ cm}^{-3}
\]
\[
K_{sat} = 40.540 \text{ cm d}^{-1}
\]
\[
\alpha = 0.01715 \text{ cm}^{-1}
\]
\[
l = -0.114
\]
\[
n = 1.442
\]

Bulk density = 1.541 g cm$^{-3}$

The applied thermal characteristics:

<table>
<thead>
<tr>
<th>material</th>
<th>lambda ($W m^{-1} K^{-1}$)</th>
<th>C ($J m^{-3} C^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>dry air</td>
<td>0.02245</td>
<td>1.255E+0003</td>
</tr>
<tr>
<td>vapor</td>
<td>0.02750</td>
<td>1.255E+0003</td>
</tr>
<tr>
<td>water</td>
<td>0.05908</td>
<td>4.180E+0006</td>
</tr>
<tr>
<td>clay</td>
<td>2.91240</td>
<td>1.920E+0006</td>
</tr>
<tr>
<td>quartz</td>
<td>8.48760</td>
<td>1.920E+0006</td>
</tr>
<tr>
<td>organic material</td>
<td>0.24960</td>
<td>2.880E+0006</td>
</tr>
</tbody>
</table>

The table with soil physical data:

<table>
<thead>
<tr>
<th>Theta h (-) (cm)</th>
<th>K (cm d$^{-1}$)</th>
<th>lambda ($W m^{-1} K^{-1}$)</th>
<th>C ($J m^{-3} C^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
<td>-1.930064E+0006</td>
<td>5.930075E-0013</td>
<td>3.817356E-0001</td>
</tr>
<tr>
<td>0.020</td>
<td>-1.927886E+0005</td>
<td>5.063941E-0010</td>
<td>3.979552E-0001</td>
</tr>
<tr>
<td>0.030</td>
<td>-4.024853E+0004</td>
<td>5.445943E-0008</td>
<td>4.127266E-0001</td>
</tr>
<tr>
<td>0.040</td>
<td>-1.609637E+0004</td>
<td>5.627864E-0007</td>
<td>4.262010E-0001</td>
</tr>
<tr>
<td>0.050</td>
<td>-1.930064E+0006</td>
<td>5.930075E-0013</td>
<td>3.817356E-0001</td>
</tr>
<tr>
<td>0.060</td>
<td>-1.927886E+0005</td>
<td>5.063941E-0010</td>
<td>3.979552E-0001</td>
</tr>
<tr>
<td>0.070</td>
<td>-4.024853E+0004</td>
<td>5.445943E-0008</td>
<td>4.127266E-0001</td>
</tr>
<tr>
<td>0.080</td>
<td>-1.609637E+0004</td>
<td>5.627864E-0007</td>
<td>4.262010E-0001</td>
</tr>
<tr>
<td>0.090</td>
<td>-1.930064E+0006</td>
<td>5.930075E-0013</td>
<td>3.817356E-0001</td>
</tr>
<tr>
<td>0.100</td>
<td>-1.927886E+0005</td>
<td>5.063941E-0010</td>
<td>3.979552E-0001</td>
</tr>
<tr>
<td>0.110</td>
<td>-4.024853E+0004</td>
<td>5.445943E-0008</td>
<td>4.127266E-0001</td>
</tr>
<tr>
<td>0.120</td>
<td>-1.609637E+0004</td>
<td>5.627864E-0007</td>
<td>4.262010E-0001</td>
</tr>
</tbody>
</table>

31
5.6 Inside the program

5.6.1 Introduction

The program HERCULES has been written in Delphi. The graphs are made using the TeeChart modules, written by David Berneda and available on Internet. First some graphs will be shown in this section that show the design of the program. Then the different objects will be described, together with their interaction.

5.6.2 Design

The general process description is presented in Fig. 1. Here the interaction between the user and the program HERCULES can be seen that was described in the previous sections. The user enters the soil texture data and the values of the thermal properties (of the constituents), and the program returns the hydraulic and thermal characteristics.

![Diagram](image)

Fig. 1 General process description of the HERCULES computer program

The right-hand circle, representing the program HERCULES, has been zoomed in and shown in more detail in Fig. 2. In this figure the circles represent processes, the open boxes represent so-called data stores and the arrows indicate transfer of data. The calculation procedure in HERCULES is straightforward. The soil texture data are fed into the PTF’s to obtain the Mualem-Van Genuchten parameters. These parameters are fed into the Mualem-Van Genuchten equations to obtain the hydraulic characteristics of the soil. They are also applied together with the thermal properties of the constituents of the soil to obtain the thermal characteristics by means of De Vries’ equation.
5.6.3 Objects

As Delphi is an object-oriented programming language, the design and implementation are based upon different objects. These objects and their mutual relationships will be discussed in this section. It is beyond the scope of this report to present the objects in full detail. Basically, four objects have been distinguished (Table 5).

Fig. 2 Detailed description of the HERCULES computer program. The circles represent processes, the open boxes represent data stores
Table 5 The Objects and a short description of their functionality

<table>
<thead>
<tr>
<th>Name</th>
<th>Descriptions</th>
</tr>
</thead>
<tbody>
<tr>
<td>PTF</td>
<td>All data and calculation for the Pedotransfer functions.</td>
</tr>
<tr>
<td>GenObj</td>
<td>All calculations and data necessary for the evaluation of the Van Genuchten equations.</td>
</tr>
<tr>
<td>HeatObj</td>
<td>Functions and parameters of Van Genuchten equations.</td>
</tr>
<tr>
<td>Table</td>
<td>All data required for the calculation of the thermal conductivity and thermal capacity. The calculations necessary to obtain these data.</td>
</tr>
</tbody>
</table>

The units
The objects described in the previous section have been translated into units. Some units are added from the Delphi environment, creating the required objects for communication with the screen or to perform some mathematical operations (Table 6).

Table 6 The units in the program HERCULES

<table>
<thead>
<tr>
<th>Unit-name</th>
<th>Object</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pages</td>
<td>Pages</td>
<td>Communication between user and computer</td>
</tr>
<tr>
<td>Pedotran</td>
<td>PTF</td>
<td>Pedotransfer functions</td>
</tr>
<tr>
<td>Genucht</td>
<td>GenObj</td>
<td>Functions and parameters of Van Genuchten equations</td>
</tr>
<tr>
<td>Heat</td>
<td>HeatObj</td>
<td>Parameters and calculations for heat conductivity and capacity</td>
</tr>
<tr>
<td>Tables</td>
<td>Table</td>
<td>Creation and storage of tables, output to file</td>
</tr>
<tr>
<td>Math</td>
<td>-</td>
<td>Some additional mathematical functions</td>
</tr>
</tbody>
</table>

The interaction between the units is presented in Fig. 3, where the arrows should be read as ‘is used by’. It can be seen from this figure that the unit Pages is the heart of the system, using the other units as required.
Fig. 3 Schematic view of the interactions between the units in the HERCULES computer model
References


