Soil physical data and modeling soil moisture flow

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Abstract

The main objectives of this study were to describe soil physical functions in a mathematically more accurate way, to investigate the soundness of the Staring Series soil physical database, to develop and apply a new 1-D soil moisture flow simulation model and to expand the Staring Series with data on coarse textured soils.

It appeared that a cubical splines method using a Mean Distance from Point to Line (MDPL) object function significantly increases fitting results of soil moisture and hydraulic conductivity data compared with other approaches currently in use.

A detailed analysis of the well-known Staring Series reveals that samples grouped into a single Staring Series class often show large differences in hydrological behaviour. Furthermore, differences between the Staring Series classes are often not statistically significant, indicating that grouping of samples should be done according to other criteria than texture and organic matter alone.

A new 1-D soil moisture flow model has been developed containing several unique features, like the cubical splines method and different irrigation criteria.

For a series of coarse sand mixtures soil physical properties were determined and hydrologically evaluated. Small differences in textural composition may lead to large differences in irrigation requirements.

Additionally, a software package has been developed to visualize 2-D soil water content changes in time as animated movies. The software package has been tested and used for multiple datasets from the Netherlands.

I dedicate this thesis to my wife and children

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After three years ‘temporary’ was changed into ‘permanent’. The present head of our team, Arie van Kekem, deserves my gratitude for his cooperation and willingness to allow me preparing the papers for this Ph.D.-thesis. I appreciate the understanding of my colleagues and project leaders (Hans Kros, Rick Wiegers, Jaco van de Gaast, Henk Vroon, Harry Massop, Jan van Bakel, Bram de Vos, Marius Heinen, Erik van den Elsen) for the sometimes delayed delivery of project results. I have been often too busy submitting papers to scientific journals and reusing them thereafter.

My colleagues Louis Dekker and Klaas Oostindie stimulated me and taught me a lot of things about field work, laboratory work and the influence of water repellency on moisture flow. We jointly published a whole series of applied and scientific papers and reports during the past few years. On the other hand, sometimes our colleagues could not understand our laughing and teasing each other. I am also grateful to Klaas for making the majority of the figures in this thesis. Louis has applied his tremendous reviewing skill to all the papers and came up with a lot of good suggestions for improvements. Klaas and Louis, thanks for these pleasant years!

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Contents

1 Introduction

1.1 Background

Soil moisture flow is an essential process in our environment. It is of importance to us because i) crops need soil moisture to grow, ii) it determines the workability of a soil, iii) it is the main transport medium for solutes, plant nutrition, pesticides and pollutants, iv) it influences surface runoff and thus flooding hazard and the need for surface water control, and v) part of our drinking water is obtained from the groundwater. For all of these reasons, it is important to understand the process of soil moisture flow and solute transport, both in the unsaturated and the saturated part of the soil. Besides doing laboratory and field studies, also simulation models are used to further understand flow and transport behavior and to perform scenario analyses.

1.2 Types of numerical models

Up to the 1990's the majority of numerical models simulated one-dimensional (i.e. vertical) moisture flow only. These one-dimensional models can be divided into two main categories (see e.g.Bastiaansen et al., 2009; Ranatunga et al., 2008): bucket models (Smith, 1992; Allen et al., 1998; Droogers et al., 2001; Prajamwong et al., 1997; De Laat, 1976), and models based upon the Richards' equation (Hansen et al., 1990; Khaleel and Yeh, 1985; Simunek et al., 1998; Van Dam et al., 1997a; Van Dam et al., 1997b; Belmans et al., 1983; Feddes et al., 1978; Vanclooster et al., 1994; Kroes and van Dam, 2003; Kroes et al., 2008; Van Dam et al., 2008). Nowadays more and more two- (e.g. Heinen, 1997; Vogel, 1997; Simunek et al., 1999) and three-dimensional models (e.g. Russo et al., 1998) are available to potential users. Generally, these types of models are data input demanding and as such not always applicable in practice. For instance, when using models, either 1-, 2- or 3-dimensional ones, boundary conditions need to be described. Meteorological data (e.g. precipitation and evaporation), drainage data (e.g. distance, depth, and resistance), and regional data (seepage or percolation) should be available at the required temporal scale.

Furthermore, soil systems need to be parameterized when using hydrological simulation models. The degree of parameterization depends upon the complexity of the soil system and the required accuracy of the model output. To parameterize soil systems, information is needed regarding regulating soil physical properties like the water retention function and the hydraulic conductivity characteristic of the distinguished soil layers.

1.3 Description of soil physical properties

Knowledge of soil hydraulic properties is essential for proper understanding and evaluation of the physical and chemical processes involved in flow of water and transport of dissolved salts and pollutants through soil systems (Al-Jabri et al., 2002; Si et al., 1999). Reliable results from numerical models of water flow and solute transport are critical for use by regulatory agencies. The accuracy of predictions is often limited by, among other things, the adequacy of hydraulic property estimations (Mertens et al., 2005; Sandhu, 2003; Wesseling et al., 2008c). These relationships are strongly non-linear and different for each soil layer considered. Many analytical equations have been developed to describe these relationships in a simple way (see Wesseling et al., 2008b for more details) while different closed-form expressions are summarized by Leij et al. (1997), Leong and Rahardho (1997) and many others.

The most-widely used method is the one where the relationships are described by the Mualem-Van Genuchten equations (Van Genuchten, 1980). The Mualem – Van Genuchten equations describe both the soil moisture retention curve and the hydraulic characteristics with six parameters: a fitted matching point for the hydraulic conductivity at saturation (K_0, [$L.T^{-1}$]), the saturated moisture content θ_s [L^3L^{-3}], the residual moisture content θ_r [L^3L^{-3}], a parameter α [L^{-1}] which is related to the inverse of the air entry suction value; a parameter n which is a measure of the pore-size distribution; and l, a pore connectivity factor that is normally assumed to be 0.5. Usually there is a discrepancy between the measured saturated value K_{sat} and the fitted value of K_0, indicating that preferably the measured K_{sat}-value should be used.

The sensitivity of soil moisture flow to the soil physical parameters has been studied by several authors using numerical models (e.g. Sandhu, 2003; Simunek and van Genuchten, 1996). Usually a sensitivity analysis is performed by varying just one or two parameters and evaluating the effect on model output, see e.g. Hari Prasad et al. (2001). Rocha et al. (2006) showed that calculations on subsurface flow in furrows was most sensitive to changes in n and in θ_s. In a study by Lu and Zhang (2002) it was discovered that n was the most sensitive parameter, followed by α and K_s. Others have applied a Monte-Carlo analysis to study the effects of soil physical parameters on moisture flow (e.g. Lu and Zhang, 2002; Mertens et al., 2005).

1.3.1 Measuring and estimating soil physical properties

To obtain the parameters of the Mualem-Van Genuchten equations from laboratory data, the curves should be fitted through a number of measured points of the soil moisture retention and hydraulic conductivity relationships. One of the most commonly used fitting programs is RETC (Van Genuchten et al., 1991), which is based upon the Marquardt-algorithm (Marquardt, 1963). Due to the strong non-linear form and the complexity of the Van Genuchten equations it is difficult to estimate in advance the influence of each parameter on the soil moisture retention and hydraulic conductivity curves, and thus on the computed soil water content or pressure head.

Different methods exist to measure the soil physical relationships in the field or in the laboratory (Ahuja et al., 1980; Boels et al., 1978; Bouma and Denning, 1972; Bouma et al., 1971; Bresler et al., 1978; Kool and Parker, 1987a; Kool et al., 1987; Stolte and Veerman, 1990; Wind, 1966). The laboratory or field measurements are often tedious and time consuming, and involve considerable uncertainty due to spatial heterogeneity of the soil system, disturbances during sampling and delicate measurement procedures (Bodhinayake et al., 2004; Shani, 1995).

There are also many in situ methods for direct estimation of the soil hydraulic functions. Examples include the crust method, where steady flux is imposed at the soil surface (Hillel and Gardner, 1970), the instantaneous profile method (Watson, 1966), and the unit gradient internal drainage approach (Libardi et al., 1980). Although relatively simple in concept, such direct methods have a number of limitations that significantly limit their use in practice. The main limitation is that they tend to be very time consuming due to the need to adhere to relatively strict initial and boundary conditions (Simunek and van Genuchten, 1996). Another limitation, especially in soils with low potential values, is that steady-state conditions are reached only after a significant amount of time due to flow dependence on hydraulic conductivity (Zhang, 1998). Measured values of saturated conductivity may be up to 30% below the actual value due to air entrapment (Zlotnik et al., 2007).

Another way is to use parameter estimation methods to determine soil hydraulic properties (Russo et al., 1991). Inherent to parameter estimation is the assumption that soil hydraulic properties may be described by a relatively simple deterministic model containing a small number of unknown parameters (Russo et al., 1991; Shani and Gordin-Katz, 1998). Contrary to the previously mentioned direct methods, parameter estimation with a predefined hydraulic model does not impose any strict requirements on the initial and boundary conditions of the measured system. Experimental methods based on the parameter estimation approach usually require less time and labour than direct methods and thus enable a larger number of measurements. This is especially important for the in situ characterization of large or heterogeneous sites (Russo et al., 1991). Inverse modelling is a parameter estimation approach frequently used in soil physical studies, for instance to estimate values from inverse modeling of soil moisture flow (Butters and Duchateau, 2002; Jhorar et al., 2001; Roulier and Jarvis, 2003; Sonnleitner et al., 2003; Yeh, 1986; Thomasson et al., 2006). In some publications the inverse modelling includes both moisture flow and solute transport (e.g. Abbasi et al., 2003; Bumgarner and McCray, 2007). Another example of inverse modeling is presented by Bumgarner and McCray (2007) who calculated the hydraulic conductivity of a waste water zone using the Hydrus-1d model.

Also, soil physical characteristics can be obtained in the field by application of infiltrometer measurements and a numerical model in combination with optimization techniques as described by Schwartz and Evett (2003) and by Lazarovitch et al. (2007).

1.3.2 Use of pedotransfer functions

Alternatively, soil physical relationships can be derived on the basis of other related soil properties using pedotransfer functions, e.g. using particle size distribution, bulk density and/or organic matter content data (Ahuja et al., 1988; Alexander and Skaggs, 1987; Bloemen, 1980; Bruce, 1972; Minasny and McBratney, 2007; Schuh and Bauder, 1986; Wösten et al., 2001a, Zacharias and Wessolek, 2007). Pedotransfer functions can be categorized into two main groups: i) class pedotransfer functions and ii) continuous pedotransfer functions. Class pedotransfer functions calculate hydraulic properties for a textural class (e.g. sand) by assuming that similar soils have similar hydraulic properties. Continuous pedotransfer functions use measured grain size distributions to provide continuously varying hydraulic properties across the textural triangle (Wösten et al., 2001a). Some researchers apply neural networks to obtain pedotransfer functions (Manyame et al., 2007; Schaap and Leij, 1998).

Although pedotransfer functions are sometimes seen as the bridge between pedology and hydrology and are gaining in popularity (Elsenbeer, 2001; Minasny et al., 1999; Nemes, 2003; Pachepsky et al., 2006; Schaap and Leij, 1998; Schaap et al., 2001; Stolte et al., 1996; Van Alphen et al., 2001), it has been shown that pedotransfer functions developed for one location are not always applicable for other locations (Li et al., 2007). Arya et al. (1999) show that it is possible to obtain the soil water retention curve from the particle-size distribution curve. New techniques have been introduced, e.g. by Nemes et al. (2006) who showed that the Nonparametric Nearest Neighbour Technique can be used to derive soil water retention data from textural data. Rasiah and Aylmore (1998) show that the parameter n of the Mualem-Van Genuchten equation is strongly determined by the bulk density of the soil. A comparison of the results of three different pedotransfer functions applied on a Niger soil has been presented by Manyame et al. (2007). It should be recognized that the usefulness of any statistical function is limited to the data population used in the development of this function. Therefore, the empirical nature of PTFs warrants their best use as starting points for quick and economic estimations of necessary model input parameters, particularly when a large number of hydraulic property data are required, making then more suitable for regional-scale studies rather than site-specific applications (Lin et al., 1999).

1.3.3 Available soil physical databases

Both raw data of soil physical relationships and more generic pedotransfer functions can be found in different databases like the Staring Series (Wösten, 1987; Wösten et al., 2001b), the Priapus database (Stolte et al., 2007; Stolte et al., 2009), the UNSODA database (Nemes et al., 2001) and the Hypres database (www.macaulay.ac.uk/hypres/; Wösten et al., 1998). As these databases are being used by many researchers in many different projects and studies (De Vries et al., 2008), it is of the greatest necessity that these databases provide accurate information to ensure sufficient quality and reliability for the end-users.

1.4 Objectives of the study and outline of this thesis

The main objectives of this study were: to describe soil physical functions in a mathematically more accurate way, to investigate the soundness of the Staring Series soil physical database, to expand it with data on coarse textured soils, and to develop and apply a new 1-D soil moisture flow simulation model. For this purpose, the following research activities were defined:

- *Describing the soil physical relationships in a mathematically more accurate way*

As mentioned earlier, the (physically based) Mualem-Van Genuchten equations are probably the most widely-used method of describing the soil physical relationships for use in numerical modeling. They describe the soil moisture retention curve and the soil hydraulic conductivity with six parameters. A fitting procedure is required to obtain the parameter values of the equations from the measured data. However, so far it is not always possible to fit satisfactory curves through the measured data derived in the laboratory or the field. Therefore, another mathematical approach is needed to describe a continuous function through the measured data. Results of this work are presented in Chapter 2.

- *Investigating the validity of clustering data from soil samples into soil physical classes*

Up to now, soil samples with similar soil textural properties are often combined into a single soil physical class. All raw data from these soil samples are then used to derive averaged soil physical functions for this specific soil class. While this may seem to be a logical procedure, enabling people to quickly find and use soil physical properties for a standard soil physical unit, uncertainty exists regarding the reliability of the results from this approach. Therefore, a critical investigation has been executed to evaluate the effects of this procedure upon computed hydrological regimes of individual samples versus "averaged" soil physical classes. Results are described in Chapter 3.

- *Model development*

To simulate flow in high spatial and temporal resolution in (non-structured, rigid) porous media, a model is needed that is capable of computing one-dimensional water flow with i) high accuracy; ii) the ability to describe soil physical relationships accurately and in different ways; iii) the use of extremely small time intervals; iv) the ability of storing model output efficiently, and v) the ability to tabulate and graphically visualize model output. As none of the available models in our working environment fulfilled all of these requirements, an alternative simulation model was built. The new software package for simulating moisture flow in soils is presented in Chapter 4.

- *Determining soil physical properties of coarse textured mixtures*

While much research has been devoted to the hydrologic behavior of relatively fine-textured soils, little attention has been paid to water movement through coarse-textured soils, such as those found on sand dunes and glacial outwash plains. These deposits can be found around the world, sometimes having limited possibilities for agricultural production due to their usually poor fertility and low water holding capacity. A search for scientific papers and data of soil physical properties of coarse materials did not yield any significant results. Therefore, a series of soil samples were prepared in the laboratory to determine the related soil physical properties and compare the different mixtures from a hydrological point of view using the newly developed simulation model. Results of these activities are described in Chapter 5.

- *Computing irrigation requirements of golf greens*

Coarse-textured soils are frequently used for the construction of golf greens because of their good drainage characteristics and low risk of compaction. Golf greens are very often constructed using sand brought in from elsewhere, with properties according to United States Golf Association (USGA) specifications. These specifications contain requirements on sand fractions to be used as well as rootzone construction guidelines (USGA Green Section Staff, 2004). Even though soil texture and potential amendments greatly affect soil water movement, these recommendations were never hydrologically evaluated using advanced simulation models. Depending on the geographical location of a golf course and the climatic conditions, water required for irrigation can be as high as 50.000 to 100.000 m^3y^{-1}. Therefore, an urgent need exists to study effects of different root zone mixtures upon the irrigation requirements of golf greens. Obtained results are discussed in Chapter 6.

- *Visualizing measured moisture contents in two dimensions*

Despite the improvement of numerical models, field measurements remain of great importance for researchers. The reasons are twofold: i) all models should be calibrated and validated, and ii) field measurements give additional and new insights in physical processes affecting water flow, e.g. the effects of soil layering, hysteresis, water repellency, and swelling and shrinking. Nowadays, more and more researchers use multiple measurement devices to unravel process mechanisms related to infiltration and movement of water through soils. Large datasets are difficult to interpret at once, so visualization can be very effective. For that purpose, a special software package has been developed which is described in Chapter 7.

2 Describing the soil physical characteristics of soil samples with cubical splines

The Mualem-Van Genuchten equations have become very popular in recent decades. Problems were encountered fitting the equations' parameters through sets of data measured in the laboratory: parameters were found which yielded results that were not monotonically increasing or decreasing. Due to the interaction between the soil moisture retention and the hydraulic conductivity relationship, some data sets yield a fit that seems not to be optimal. So the search for alternatives started. The cubical spline approximation of the soil physical characteristics appears to yield good approximations. Software was developed to fit the spline-based curves to sets of measured data. Five different objective functions have been tested and their results compared for four different data sets. It is shown that the well-known least-square approximation does not always perform best. The distance between the measured points and the fitted curve, as can be evaluated numerically in a simple way, appears to yield good fits when applied as a criterion in the optimization procedure. Despite an increase in computational effort, this method is recommended over others.

Adapted from

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Describing the soil physical characteristics of soil samples with cubical splines.

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2.1 Introduction

The capacity of digital computers has increased enormously in recent years. This means more computations can be performed in less time. Now it becomes possible to design and run programs on a personal computer or minicomputer that previously could run only on a mainframe. In the field of unsaturated soil moisture flow this has resulted in models getting more and more detailed.

Up to a decade ago the majority of numerical models simulated one-dimensional (i.e. vertical) moisture flow only (see e.g. Hansen et al., 1990; Simunek and van Genuchten, 1996; Van Dam et al., 1997a; Van Dam et al., 1997b). Nowadays more and more two- (e.g. Heinen, 1997; Vogel, 1997; Simunek et al., 1999) and three-dimensional models (e.g. Russo et al., 1998) are available for potential users. See the website of the International Groundwater Modeling Center (http://www.mines.edu/igwmc/software/) for more models on groundwater flow and their availability. Most of these models simulate transient moisture flow based upon the Richards' equation.

Whatever number of dimensions is considered and whatever equation is applied, some soil physical relationships should be known. In case of the Richards' equation, these relationships are the soil moisture retention curve (a relationship between pressure head and moisture content) and the hydraulic conductivity characteristic (a relationship between the hydraulic conductivity and the pressure head). Many researchers do not take soil samples themselves but depend on data found in literature or in available databases such as the Staring Series (Stolte et al., 2007; Wösten, 1987; Wösten et al., 2001b), the UNSODA database (Nemes et al., 2001) or the Hypres database (see http://www.macaulay.ac.uk/hypres/; Wösten et al., 1998). Therefore it is of the greatest necessity to describe the measured relationships the best way possible.

A lot of attempts have been made to describe the soil physical relationships with analytical equations. Nowadays one of the most widely-used methods is the so-called Mualem-Van Genuchten equation (Van Genuchten, 1980). It describes both the soil moisture retention curve and the hydraulic conductivity relationship using only 6 parameters. This simplicity is at the same time the weakness of the method: not all combinations of curves can be approximated adequately. Software is available to estimate the 6 parameters of the equations using the measured points (Stolte, 1997; Van Genuchten et al., 1991). This software is usually based upon the least square approximation and some second order optimization technique. The main disadvantage of the least square approximation is that it usually takes into account the vertical distance between the measured point and the fitted curve. The second order optimization techniques yield a fast way to a (possibly local) minimum. This requires quite some numerical calculations since the second order derivative of a function, the Hessian matrix, should be evaluated numerically. Still, it often appears that not all combinations of soil water retention curves and the hydraulic conductivity relationship can be adequately approximated.

Therefore, several authors have presented the approximation of the relationships using polynomials or cubical splines (e.g. Bitterlich et al., 2004; Erh, 1972; Kastanek and Nielsen, 2001; Prunty and Casey, 2002). Despite the fact that these publications show the power and capability of the spline functions, application has not yet been very popular in research. Therefore this study shows another spline approximation of the soil physical relationships. For this purpose software was written to fit curves through the points measured in the laboratory. This software is based upon some simple direct-search optimization techniques. In most publications the spline-functions are fitted using the least square of deviations criterion. Despite the usefulness of this method, there are other and better criterions known in mathematics. In this chapter five different objective functions are described and tested on four soil samples. Results are also compared to approximations obtained with the commonly-used RETC-program (Van Genuchten et al., 1991).

2.2 Material and methods

To understand the importance of reliable soil physical relationships, one should be familiar with the equations governing soil moisture flow in the unsaturated zone of the soil. This partial differential equation is presented in the next paragraph. The individual points of these relationships are usually measured in the field or the laboratory, yielding a collection of points. Plotting these points in a graph usually results in some 'clouds' of points. Several attempts have been made to develop equations that are generally applicable to describe the relationships. Some of these are mentioned in the following paragraph. The parameters of these relationships should be estimated in such a way that the curve fits the measured points in the best possible way. We choose to describe the curve by cubical splines because it can be expected that the accuracy of the derived approximation would increase. These splines are described in detail. In order to obtain the best fit of the spline-approximation through the measured points, some optimization procedure is required. The general theory of these procedures is presented. An optimization procedure can work only if there is some function it has to optimize, or in this case, minimize. Five different types of these functions are described. The optimal points of the spline curves are calculated by using these functions.

2.2.1 Soil moisture flow

Soil moisture flow in a N-dimensional system can be described by the following partial differential equation

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \left(K \nabla H \right) - S \tag{2.1}$$

where

$$\nabla = \sum_{i=1}^{N} \frac{\partial}{\partial x_i} \tag{2.2}$$

and H = total head [L]; x_i = coordinate in i^{th} direction; θ = volumetric moisture content [L^3L^{-3}]; t = time [T]; K = prevailing hydraulic conductivity [LT^{-1}]; S = sink term representing drainage flow or root extraction [T^{-1}].

Introduction of anisotropy (for 3-dimensional flow) leads to

$$K = K_{ij} = \begin{pmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{pmatrix} \tag{2.3}$$

and the total head H can be written as

$$H = h + x_3 \tag{2.4}$$

where h = pressure head [L] and x_3 = vertical position [L].

Introducing the differential moisture capacity C [L^{-1}] then yields

$$C\frac{\partial H}{\partial t} = \sum_{i=1}^{3}\frac{\partial}{\partial x_i}\sum_{j=1}^{3}K_{ij}\frac{\partial H}{\partial x_j} - S \tag{2.5}$$

with $$C = \frac{d\theta}{dH} = \frac{d\theta}{dh} \tag{2.6}$$

Both K and C-values depend on the prevailing pressure head h. To solve eq. (2.5), the C(h), K(h) and h(θ) relationships should be known. Here we focus on the K(h) and h(θ) relationships.

2.2.2 Analytical approximations of soil moisture retention and hydraulic conductivity functions

The relationships between moisture content, pressure head and hydraulic conductivity are very important to obtain a correct description of unsaturated moisture flow. They can be measured in the field or in the laboratory using different methods (e.g.Ahuja et al., 1980; Boels et al., 1978; Bouma and Denning, 1972; Bouma et al., 1971; Bresler et al., 1978; Kool and Parker, 1987a; Kool and Parker, 1987b; Stolte and Veerman, 1990; Van Dam et al., 1990; Wind, 1966). Several authors try to derive these relationships from other known soil physical data, e.g. particle size distribution and organic matter content (Ahuja et al., 1988; Alexander and Skaggs, 1987; Bloemen, 1980; Bruce, 1972; Schuh and Bauder, 1986). Several analytical functions have been developed to describe the soil-physical relationships. Excellent overviews and comparison of a lot of closed-form expressions can be found in literature (Leij et al., 1997; Leong and Rahardjo, 1997).

One of the most frequently used closed-form descriptions of the soil physical relationships is the one introduced by (Van Genuchten, 1980) who describes the K(h)- and h(θ)-relationships as S-shaped curves with only 6 parameters. It appears however that this closed-form approximation can still be improved (Fuentes et al., 1992; Fuentes et al., 1991). These equations state

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\left(1 + |\alpha h|^n\right)^m} \tag{2.7}$$

$$h = \frac{\left(\left(\frac{\theta_s - \theta_r}{\theta - \theta_r}\right)^{\frac{1}{m}} - 1\right)^{\frac{1}{n}}}{\alpha} \tag{2.8}$$

$$K = K_0 \frac{\left(\left(1 + |\alpha h|^n\right)^m - |\alpha h|^{n-1}\right)^2}{\left(1 + |\alpha h|^n\right)^{m(l+2)}} \tag{2.9}$$

with

$$m = 1 - \frac{1}{n} \tag{2.10}$$

Differentiation also yields an equation for the differential moisture capacity:

$$C_\theta = \frac{\partial \theta}{\partial h} = n \cdot m \cdot \alpha \cdot |\alpha h|^{n-1} \cdot \frac{\theta_s - \theta_r}{\left(1 + |\alpha h|^n\right)^{m+1}} \tag{2.11}$$

where h = pressure head (cm), θ = moisture content ($cm^3 cm^{-3}$), K = hydraulic conductivity ($cm\ d^{-1}$) and C = differential moisture capacity (cm^{-1}); α (>0, in cm^{-1}) is related to the inverse of the air entry suction; n (>1) is a measure of the pore-size distribution; K_s is a fitted matching point at saturation ($cm\ d^{-1}$) and l is an empirical parameter that is normally assumed to be 0.5.

Parameters for the closed-form expressions can sometimes be determined by inverse modelling (Jhorar et al., 2001; Yeh, 1986), but the majority is still derived from laboratory data. Relationships between soil physical characteristics and other soil properties (e.g. organic matter content, particle size distribution, texture etc.) are getting more and more popular as well (Elsenbeer, 2001; Minasny et al., 1999; Nemes, 2003; Schaap and Leij, 1998; Schaap et al., 2001; Stolte et al., 1996; Van Alphen et al., 2001; Wösten et al., 2001b). These are the so-called pedotransfer functions.

Instead of using a closed-form description of the soil physical relationships, sometimes the soil physical characteristics in numerical models are described by tables with data-couples, e.g. (θ,h)- and (h,K)-points. To obtain the corresponding values for data between the specified nodes, linear interpolation is applied (sometimes after taking the ^{10}log of the values). This may be the cause of some unnecessary iterations because these functions may cause 'jumps': the value of the differential moisture capacity of a point may not be continuous across such a point.

In the following sections it is assumed that we have a number of measured points of a soil-physical relationship. At this point it does not matter how these data are obtained, they are just available and assumed to be correct. They can be presented as a cloud of points in a graph. To be able to use the relationship in numerical modeling, it should be described by some function.

2.2.3 Splines

One of the most powerful mathematical methods of describing a function is the one applying splines. These are piecewise-continuous polynomials. Several types of splines have been applied in soil science, e.g. cubic splines (Hampton, 1990; Kastanek and Nielsen, 2001; Prunty and Casey, 2002) and quadratic B-splines (Bitterlich et al., 2004). Though nowadays spline interpolation is included in mathematical and statistical packages like MathLab (http://www.mathworks.com) and Statistica (http://www.statsoft.com), these packages are not generally available for researchers. Beside that, it appears that most researchers are unfamiliar with the theory of splines. Therefor this section will describe the theory of cubical splines in a general way. Splines are described by defining only a few data points. These points are sometimes called Virtual Data Points (see Kastanek and Nielsen, 2001). The function-values for points located between these Virtual Data Points are then calculated by computing the value of the spline function. Now suppose we have a series of (virtual) data pairs (x_i,y_i), i=1..N. We assume the series is ordered by x, i.e. $x_i < x_{i+1}$ and we focus on the interval $[x_i,x_{i+1}]$. Then linear interpolation in that interval gives the interpolation formula

$$y = \alpha y_i + \beta y_{i+1} \tag{2.12}$$

where

$$\alpha = \frac{x_{i+1} - x}{x_{i+1} - x_i} \tag{2.13}$$

$$\beta = 1 - \alpha = \frac{x - x_i}{x_{i+1} - x_i} \tag{2.14}$$

Since it is piecewise linear, the equation above has a second derivative of zero in the interior of each interval and an undefined second derivative at the abscissas x_j. Now the goal of cubic spline interpolation is to get an interpolation formula that is smooth in the first derivative and continuous in the second derivative, both within an interval and at its boundaries. It is required that the second derivative varies linearly from a value y_i'' on the left to a value of y''_{i+1} on the right. In order to fulfill all these requirements, we have to introduce a cubic polynomial instead of a linear relationship. Doing so, we will have the desired continuous derivative. The polynomial should be constructed in such a way it has zero values at x_i and y_{i+1} so adding it will disagree with the values y_i and y_{i+1} at x_i and x_{i+1}. Some elementary calculus now yields the new interpolation formula:

$$y = \alpha y_i + \beta y_{i+1} + \gamma y_i^{''} + \eta y_{i+1}^{''} \tag{2.15}$$

where

$$\gamma = \frac{1}{6}\left(\alpha^3 - \alpha\right)\left(x_{i+1} - x_i\right)^2 \tag{2.16}$$

and

$$\eta = \frac{1}{6}\left(\beta^3 - \beta\right)\left(x_{i+1} - x_i\right)^2 \tag{2.17}$$

It is easy to check that y” is the second derivative of the interpolating polynomial. Remembering that α, β, γ and η are functions of x, it is possible to find the derivative of y with respect to x:

$$\frac{dy}{dx} = \frac{y_{i+1} - y_i}{x_{i+1} - x_i} = \frac{3\alpha^2 - 1}{6}\left(x_{i+1} - x_i\right)y_i^{''} + \frac{3\beta^2 - 1}{6}\left(x_{i+1} - x_i\right)y_{i+1}^{''} \tag{2.18}$$

and the second derivative

$$\frac{d^2y}{dx^2} = \alpha y_i^{''} + \beta y_{i+1}^{''} \tag{2.19}$$

The problem now is that the values of the $y^{”}_i$ ’s are supposed to be known but are not. However, up to now it wasn’t required for the first derivative to be continuous across the boundary between two intervals. The key idea about cubic splines is to require this continuity and to use it to get equations for the second derivatives.

The required equations are obtained by setting the first derivative for $x=x_i$ in $[x_{i-1}, x_i]$ equal to the same equation for $x=x_i$ in $[x_i, x_{i+1}]$. After some rearrangement this gives for each $i \in [2..N-1]$:

$$\frac{x_i - x_{i-1}}{6} y''_{i-1} + \frac{x_{i+1} - x_{i-1}}{3} y''_i + \frac{x_{i+1} - x_i}{6} y''_{i+1} = \frac{y_{i+1} - y_i}{x_{i+1} - x_i} - \frac{y_i - y_{i-1}}{x_i - x_{i-1}} \qquad (2.20)$$

These are N-2 linear equations in the N unknowns y''_i, i=1..N. For a unique solution we need to specify two further conditions, typically taken as boundary conditions at x_1 and x_N. The most common ways to do this are either to set one or both of the boundaries to zero or calculate the first derivative to have a specified value on either or both boundaries.

After calculating the second derivatives once, their values should be stored and the interpolation between points can rapidly be performed according to Eq. (2.15), see also Press et al. (1986) and Erh (1972).

2.2.4 Parameter estimation

In the previous section the spline approximation has been described. But how can we obtain the values of the Virtual Data Points (x_i,y_i) that fit the measured data in the best possible way? For that purpose we need the parameter estimation or optimization techniques. These will be presented in general in this section.

2.2.4.1 The problem

Most systems and relationships in soil physics can be described by a mathematical function f, having some parameters p. Depending on the value of the parameter set $\underline{p}$, a series of input data (state variables) $\underline{x}$ (a vector), applied to the system described by f and assuming some initial and boundary conditions, produces a series of output data $\underline{\hat{y}}$ (a vector as well). Written in a mathematical form

$$\underline{\hat{y}} = f\left(\underline{p},\underline{x}\right) \qquad (2.21)$$

where $\underline{x}$ = vector with independent (state) variables; $\underline{p}$ = parameter vector; $\underline{\hat{y}}$ = vector with output data obtained from the combination of the vector with state variables $\underline{x}$ and the vector with parameters $\underline{p}$; N_x = number of state variables (dimension of $\underline{x}$); N_y = number of output data (dimension of vector $\underline{y}$); N_p = number of parameters (dimension of vector $\underline{p}$); f = mathematical function that describes the conversion of input data x to output data y, depending on the parameter set $\underline{p}$.

In this context the function f may vary from a simple relation to a very complex set of equations. See e.g. (Vrugt et al., 2002) and (Mertens, 2003) for more details about parameter identificability and parameter estimation strategies in subsurface hydrology.

In some cases the parameter vector $\underline{p}$ is known beforehand. Then the output vector $\underline{\hat{y}}$ of the function f can be seen as an accurate response to the data in the input vector $\underline{x}$, presuming the system is described correctly by f. However, this is not always the case. Presuming again that f presents a correct description of the system under consideration, one has to vary the values in the parameter vector $\underline{p}$ to obtain an output vector $\underline{\hat{y}}$ that approximates the vector $\underline{y}$ with measured values as closely as possible (calibration of parameter values). Often the parameter vector $\underline{p}$ represents physical characteristics which may be measured in laboratories or in the field, e.g. saturated hydraulic conductivity or the slope of the soil water retention curve. Usually the measurements of physical characteristics are time consuming and expensive. When f describes the system under consideration correctly, the parameter vector $\underline{p}$ can sometimes be derived from simple input-output measurements, (e.g. the one-step outflow method (Kool et al., 1985) or the multi-step method (Van Dam et al., 1990) in case of soil physical parameters). In these cases the input to the system is fully controlled and the output is measured. Knowing the input- and output vectors of the system by measurement, an attempt can be made to find the vector $\underline{p}$. The values of the parameter vector $\underline{p}$ should be set in such a way that the calculated values in the output vector $\underline{\hat{y}}$ approximate the measured values in vector $\underline{y}$ as well as possible. This is called an indirect inverse problem. The solution of the problem depends on several factors, e.g. the type of function f and the amount of parameters N_p. Several authors presented solutions of the inverse problems (Baker, 2006; Press et al., 1986; Spriet and Vansteenkiste, 1982; Tarantola, 1987). The inverse problem can be solved by one of the known optimization techniques (e.g. Baker, 2006; Cesari, 1983; Gill et al., 1981;

Luenberger, 1973; Press et al., 1986; Rust and Burrus, 1972; Van Beek and Hendriks, 1983). The problem discussed above can be stated as follows:

$$\underset{\underline{p}}{Minimize}\; g\left(\underline{p}, \underline{y}, \underline{\hat{y}}\right) \tag{2.22}$$

where g is the objective function. The value of g is not only depending on the measured ($\underline{y}$) and the calculated ($\underline{\hat{y}}$) output values, but one can implicitly take care of constrains as well. If only positive values are allowed for a parameter, negative values will yield a high value of the function (in case of a minimization procedure). Stating the problem this way, the function g should be chosen such that its value gets smaller when the calculated values approximate the measured values.

Translating the theory above to our spline problem, the vector $\underline{p}$ is considered as consisting of the x- and y-coordinates of the Virtual Data Points and the function g as being some function considering the goodness of fit, the objective function. This function will be described later.

Sometimes one is forced to apply weight functions to obtain reasonable results. Then each point is assigned a value ω and the function is calculated as

$$\gamma\left(\underline{y}, \underline{\hat{y}}\right) = \sum_{i=1}^{N_y} \omega_i g(y_i, \hat{y}_i) \tag{2.23}$$

where γ is the resulting objective function. Usually ω_i is determined by expert judgment or by trial and error. To find the optimum values of the weight function, a separate optimization procedure should be developed. In the remainder of this chapter values of the weight functions will be set to 1 (all points are equally important).

2.2.4.2 The minimization procedure

From literature many optimization procedures are known. These procedures can be divided into two main classes:

- Direct search methods. When applying these methods only the function g($\underline{y}$, $\underline{\hat{y}}$) has to be evaluated.

- Line search methods. In all of the methods belonging to this group a search for the minimum is performed where the minimum of g is expected. In most cases this direction is found by calculating the derivative g'(y,), where

$$\underline{g}'(\underline{y},\hat{\underline{y}})=\left(\frac{\partial g}{\partial p_1},\frac{\partial g}{\partial p_2},\ldots\ldots,\frac{\partial g}{\partial p_{N_p}}\right) \quad (2.24)$$

  Some line search methods take into consideration the matrix with second derivatives (the Hessian matrix) H as well. In most cases the function g can not be described analytically, so g' and H have to be evaluated numerically, requiring a large amount of function evaluations.

To obtain the results presented in the remainder of this chapter, two different direct search optimization techniques were investigated: the Simplex method (Nelder and Mead, 1965; Press et al., 1986) and the Controlled Random Search algorithm or CRS (Price, 1979). The Simplex method was chosen because it is a well-known method that has been applied in a wide range of problems. The CRS-method is known for its simplicity and has been applied with good results (Metselaar, 1999). As both methods yielded very similar results, only the results with the CRS-method are discussed.

2.2.4.3 The objective functions

In the previous sections the optimization problem has been stated and some optimization procedures have been mentioned. But what function do we have to optimize? And how do we calculate this function? Some of the many possible objective functions will be described below.

It is assumed that a number of measured data y(x,p) has to be approximated by $\hat{\underline{y}}$ = f(x,p). The function $y_i = f(x_i,p)$ is graphically represented by a geometrical figure Ω in space R^2. This may be either a straight line or some kind of complex curve (See Figure 2.1).

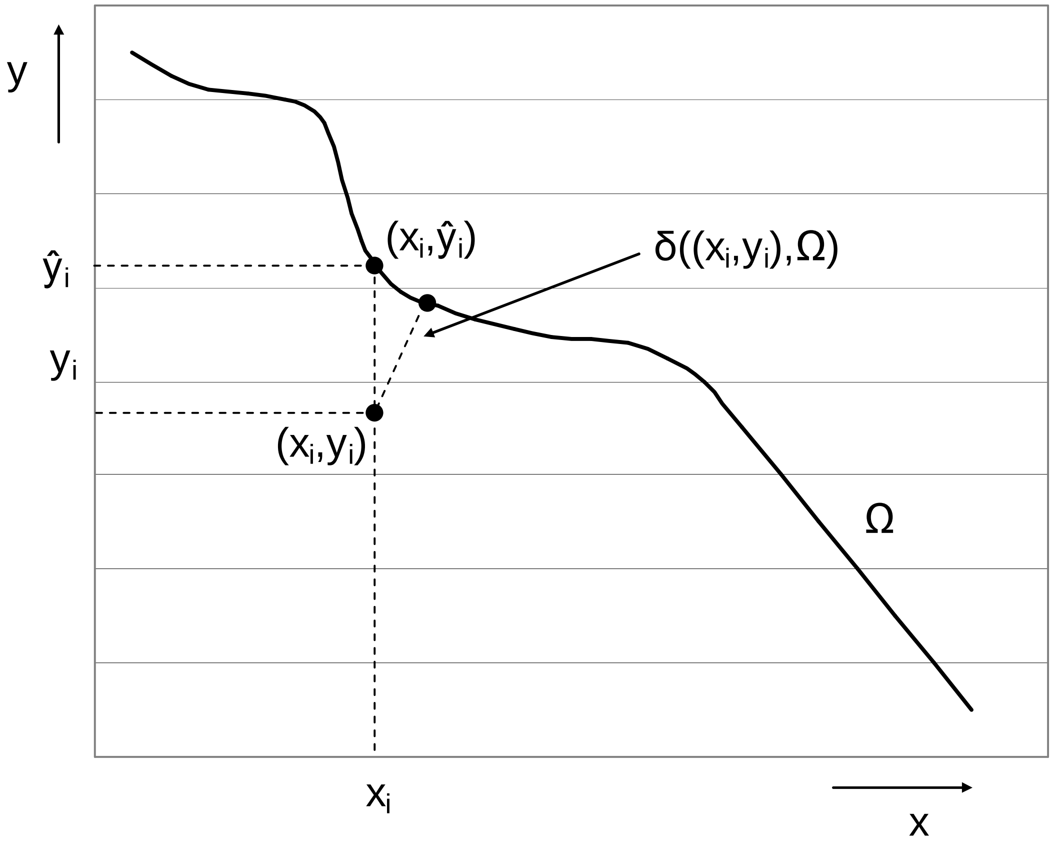


Figure 2.1 A schematic representation of a measured point (x_i,y_i), a calculated point (x_i,$\hat{y}_i$) and the distance δ between the measured point and the calculated line Ω.

- The simplest objective function is the sum of the absolute deviation between the measured value y_i and the calculated value $\hat{y}_i$ for a specified x_i. This is written as

$$g(\underline{y},\underline{\hat{y}}) = \sum_{i=1}^{N_y} |y_i - \hat{y}_i| \qquad (2.25)$$

  The main advantage of this equation is its simplicity, while one of its drawbacks is that large deviations have an extremely big influence on the results.

- The most widely used objective function is the sum of the squares of deviations:

$$g(\underline{y},\underline{\hat{y}}) = \sum_{i=1}^{N_y} (y_i - \hat{y}_i)^2 \qquad (2.26)$$

  Complete optimization theories have been developed based upon this objective function (e.g. Marquardt, 1963). The disadvantage mentioned before is even stronger in this case. This least square function has been applied regularly when describing soil physical properties (e.g. Bruckler et al., 1987; Kool and Parker, 1988; Stephens and Rehfeldt, 1985).

- If the values of y differ some magnitudes it is advisable to consider the relative error instead of the absolute error that was taken in the previous 2 functions. Then g can be written as in

$$g\left(\underline{y},\underline{\hat{y}}\right)=\sum_{i=1}^{N_y}\frac{\left|y_i-\hat{y}_i\right|}{\left|y_i\right|} \tag{2.27}$$

  A disadvantage of this method is the fact that problems arise when y_i approaches 0. In that case an exception should be made and a different function should be taken for this point.

- Another possibility is to calculate the difference between the absolute values of the quotients of measured and calculated values

$$g\left(\underline{y},\underline{\hat{y}}\right)=\sum_{i=1}^{N_y}\left(\frac{\left|\hat{y}_i\right|}{\left|y_i\right|}+\frac{\left|y_i\right|}{\left|\hat{y}_i\right|}-2\right) \tag{2.28}$$

  The main advantage of this method is that it does not matter if the calculated value is a certain fraction higher or lower than the measured value: the contribution to the objective function is the same. This can easily be seen when the value of g is plotted against the percentage of deviation. There are two disadvantages to this method: the first one occurs when either y_i or $\hat{y}_i$ approaches 0 (division by zero), the second problem is that the possibility of different signs of y_i and $\hat{y}_i$ is not taken into account. If this sign difference occurs, an extra (large) value has to be added to the objective function to avoid this sign difference in the final solution.

- The objective function that is intuitively seen as the most correct one represents the sum of the distances from the point (x_i,y_i) to Ω.

$$g\left(\underline{y},\underline{\hat{y}}\right)=\sum_{i=1}^{N_y}\delta\left[\Omega\left(x_i,y_i\right)\right] \tag{2.29}$$

This would yield the best approximation of a line through a series of points. In practice it is hardly applied, due to the fact that it is difficult to calculate the distance between a point and a line if the line is described by a complex equation. If this is the case, calculating the distance can be viewed at as another problem of optimization: find the coordinates of the element of Ω where the distance to the point under consideration is at minimum. Application of this criterion may take a lot of extra programming. It can be considered as a Total Least Squares approach used when both x and y contain errors in a regression problem.

2.2.4.4 Goodness of fit

The most widely spread indicator for the goodness of fit is the root-mean-square error (see e.g. Prunty and Casey, 2002). This value is based upon the sum of the squares of deviations between measured and calculated values at a given x-value, mathematically written as:

$$SSQ(\underline{p}) = \sum_{i=1}^{N_y} \left(\hat{y}_i - f\left(\underline{p}, x_i\right)\right) \qquad (2.30)$$

and

$$RMSE = \sqrt{\frac{SSQ(\underline{p})}{N_y}} \qquad (2.31)$$

As we stated before, the sum of the distances from the measured point to the calculated line is a better criterion for the goodness of fit than the root of squares of deviations. Therefore we want to introduce a new criterion for the goodness of fit, the Mean Distance of Points to Line (MDPL). This can simply be calculated by

$$MDPL = \frac{1}{N_y} \sum_{i=1}^{N_y} \delta(\Omega(x_i, y_i)) \qquad (2.32)$$

2.2.4.5 Calculating the distance between a point and a line

From mathematics many equations are known to calculate the distance from a point to a straight line. Equations for some simple other line types can be found as well. But what to do with a set of spline functions fitted through a number of Virtual Data Points? This complex problem was solved numerically:

- Suppose we have data points in the range x_1 to x_{Nx}. Each x-value has a corresponding y-value.
- Divide the range into a large number (N, say 1000) of intervals. In this way we obtain N+1 values on the x-axis, say ρ_j. For each of these values we can calculate a corresponding function value σ_j by spline-interpolation.
- For each measured point (x_i,y_i) the distance to the line can now be found as the minimum value of the measured point to one of the generated points, or in an equation:

$$\delta[\Omega,(x_i,y_i)] = \min_j\left(\delta\left((x_i,y_i),(\rho_j,\sigma_j)\right)\right) = \min_j\left(\sqrt{(x_i-\rho_j)^2+(y_i-\sigma_j)^2}\right) \qquad (2.33)$$

2.2.5 Software to estimate the points of the optimal spline functions

In this Chapter methods are developed to approximate the soil physical characteristics by means of a number of cubical splines. Only a number of points of the line have to be found. Values for other points can be calculated by means of a simple cubical interpolation. Assuming the splines are described by equation (2.15), then we may consider this equation as a special form of the general equation (2.21). From the laboratory we have a number of combinations of x- and y-values (θ and h in case of soil moisture retention, h and K in case of hydraulic conductivity). The optimization techniques can now be applied to this equation to find the optimal fit for the data. Any of the objective functions described above (Eq. (2.25) to (2.29)) may be used.

The equations and methods described earlier are translated into some computer programs (all developed in Delphi 7 and running under Windows XP):

- Optim.exe is a program to i) fit a polynomial of an arbitrary degree through a number of points and ii) fit the Mualem - Van Genuchten parameters for a set of K(h) and h(θ) data.
- Spline.exe is a program to manually fit cubical splines through a dataset. The Virtual Data Points have to be entered and the program shows the interpolated values as a graph.
- Splop.exe automatically fits a spline function through a set of data.

It is essential that the fitted line is monotonic. Several authors (Bitterlich et al., 2004; Hampton, 1990) applied piecewise cubic Hermite interpolation to insure monocity. In general, one can indicate the requirement of a monotonic increasing or monotonic decreasing line. The check of being monotonic is performed by dividing the range of the x-values into a large number of intervals and checking if the corresponding y-value is higher (resp. lower) than the one corresponding to the previous x-value.

It would go too far to describe the programs in more detail here. Only results of applying Splop.exe will be discussed here.

2.3 Results and discussion

Five objective functions were tested on four different data sets. The methods described above were applied on the hydraulic conductivity relationship of two soil samples. Both the hydraulic conductivity function and the soil moisture retention curve of a soil sample were approximated. This sample was also used to show the influence of the number of Virtual Data Points on the optimal value of the objective function. Finally a comparison of the results obtained with the different objective functions is presented. Wherever applicable, the Mualem-Van Genuchten approximation of the data obtained by the program RETC (Van Genuchten et al., 1991) is shown as well. All runs with RETC were made with the same initial values (Stolte et al., 2007) and the measured points of both the soil moisture retention curve and the hydraulic conductivity characteristic were taken into account, implying that the points of the soil moisture retention curve may influence the fit of the hydraulic conductivity curve and vice versa.

2.3.1 Fitting K(h)-relationships

From a site in The Netherlands, a sandy soil sample (here referred to as 'Tox') was collected at 30-38 cm depth for soil physical determination in the laboratory. Using the evaporation method (Halbertsma and Veerman, 1994; Wind, 1966), a series of K(h)-points was obtained. These data are used here to fit an approximation with splines. All objective functions were applied and the resulting curves are presented in Figure 2.2.

It can be seen that the results obtained with eq. (2.29) represent the best fit.

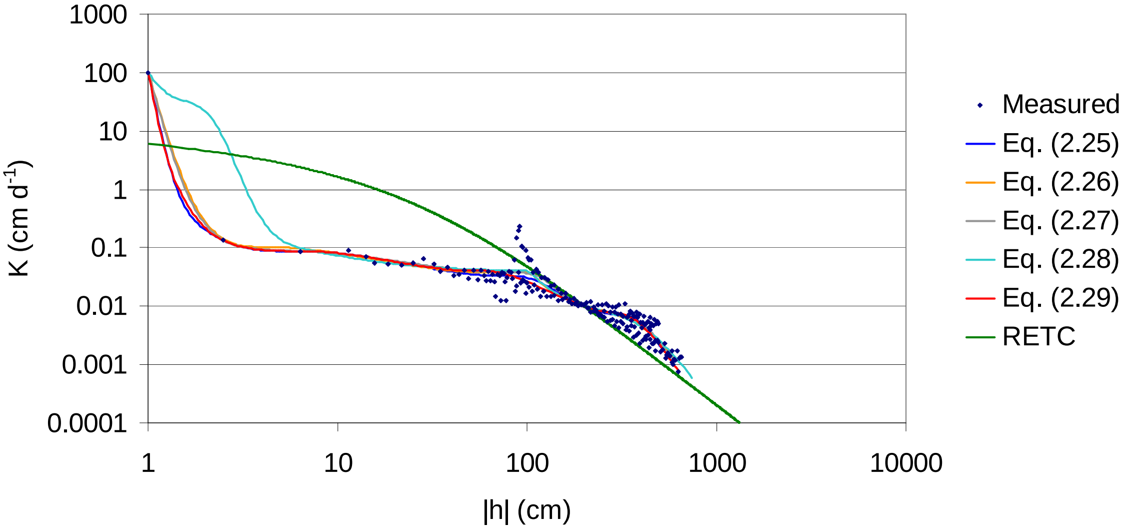


Figure 2.2 Measured hydraulic conductivity K (cm d^{-1}) as a function of the pressure head h (cm) and the optimal fits for the Tox-sample.

The quotient objective function yields a rather strange exception. It appeared that before optimizing the curve, first the ^{10}log of the y-values was taken. In this case the value is 0.1, yielding a log-value of -1. The program gets a y-value of 10, yielding a log-value of 1. Inserting these values in Eq. (2.28) yields an exact equality as the absolute values are considered. At the area with many points, the different object functions yield slightly different results also. It is clear that the RETC-fit is nowhere near the measured point for values of h > -100 cm. The conductivity at saturation (h=0) is not well approximated either. When zooming in on the range between -200 cm and -40 cm, the differences become visible (Figure 2.3).

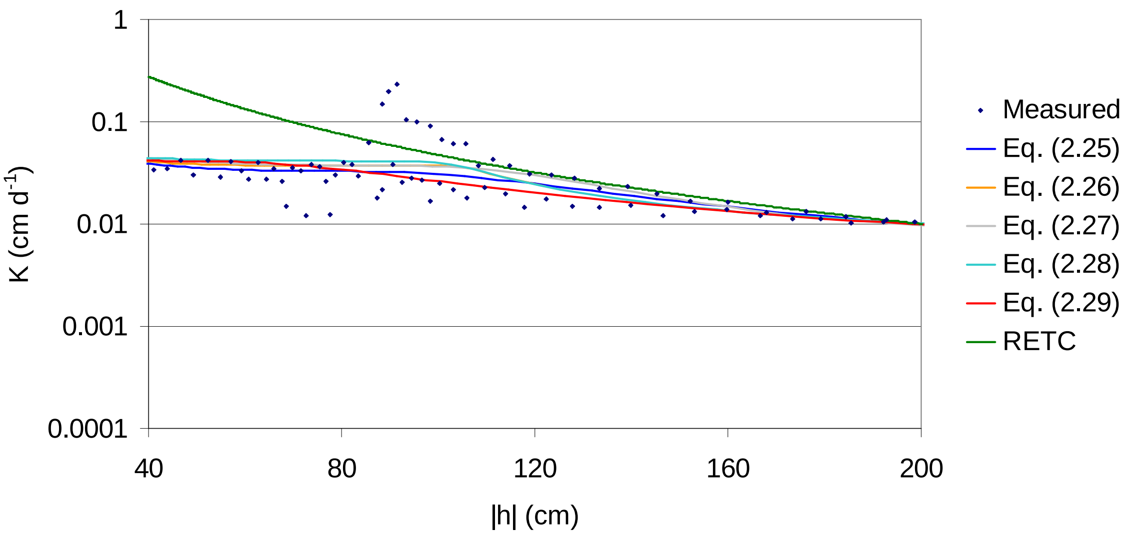


Figure 2.3 Measured hydraulic conductivity K (cm d^{-1}) as a function of the pressure head h (cm) and the optimal fits for the Tox-sample in the range of |h|=40 to |h|=200 cm pressure head.

During the past decades the soil physical characteristics of quite a lot of soil samples have been determined at Alterra, Wageningen, The Netherlands. All these data were colllected into the Priapus database recently and software was developed to make the data accessible via internet (Stolte et al., 2007). From this database another soil sample was selected to use in this study. It was a sample from Glanerbrug in The Netherlands. The sample will be referred to as kh61. This sample was selected because, at first sight, both the soil moisture retention curve and the hydraulic conductivity curve seemed to show a good fit through the measured points (Figure 2.4).

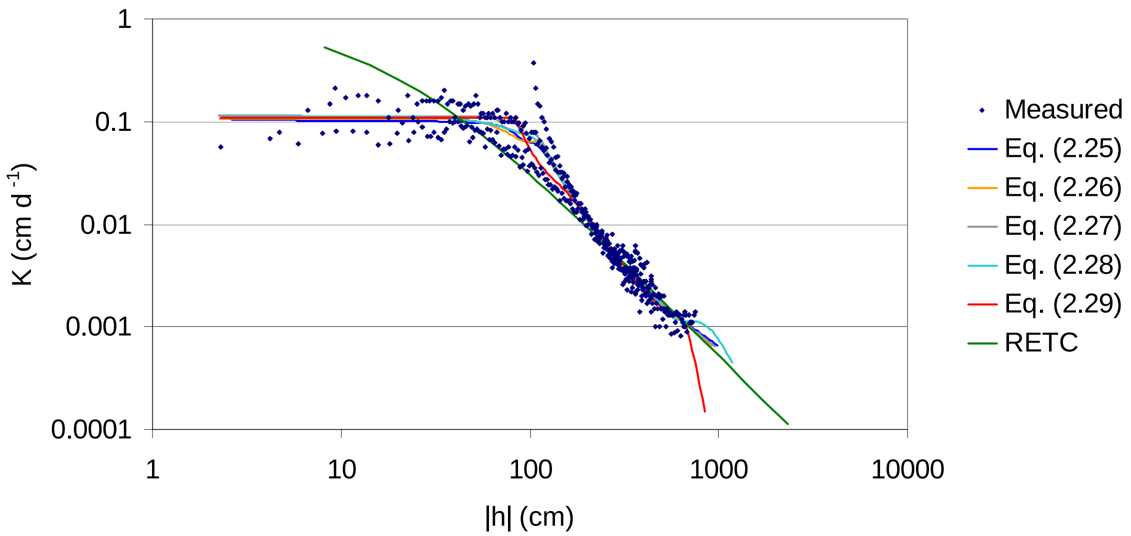


Figure 2.4 Measured hydraulic conductivity K (cm d^{-1}) as a function of the pressure head h (cm) and the optimal fits for the kh61-sample.

However, when you plot only the values in the range of pressure head values between -200 and -40 cm (Figure 2.5), it becomes clear there is a difference between the lines and that the RETC-fit will produce lower K-values than the other fits.

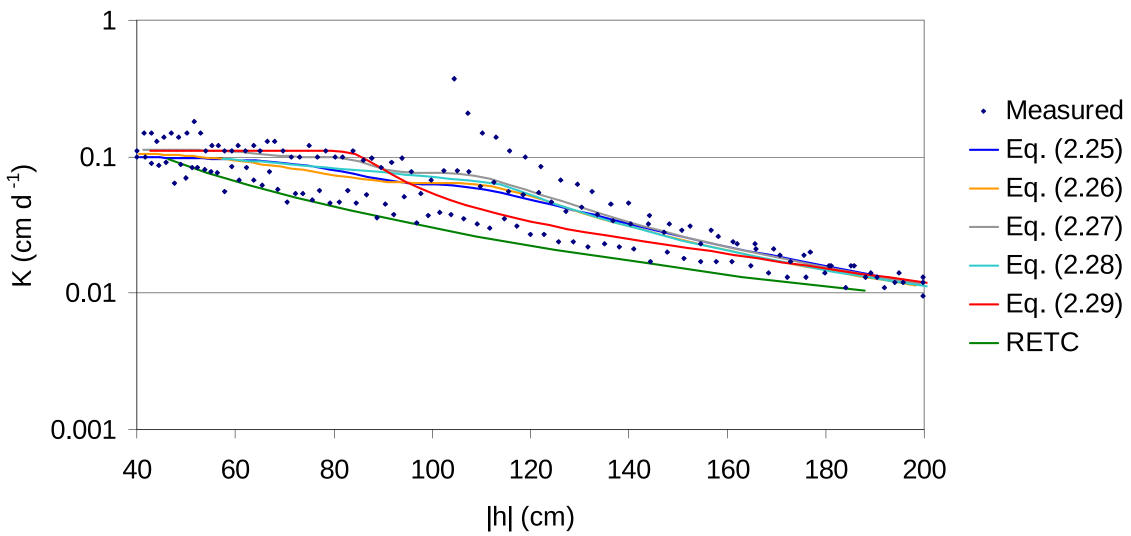


Figure 2.5 Part of the fitted curves through the measured hydraulic conductivity data of sample kh61 between pressure head values |h| =40 and |h| =200 cm.

The optimization was performed for 10 spline points. The values between these points were interpolated applying equations (2.25) to (2.29). Now an interesting question is how do these spline points differ for each objective function? In all cases we used 10 points (0..9). The values for the points of the optimal curves are presented in Table 2.1.

Table 2.1 (K-h)-points of the spline-interpolation function for each objective function with h in cm, K in (cm d^{-1}). The subscript of the h's and k's refer to the different objective functions described earlier.

i	h_{25}	k_{25}	h_{26}	k_{26}	h_{27}	k_{27}	h_{28}	k_{28}	h_{29}	k_{29}
0	2.29	$1.06 \cdot 10^{-1}$	2.27	$1.07 \cdot 10^{-1}$	2.25	$1.14 \cdot 10^{-1}$	2.31	$1.12 \cdot 10^{-1}$	2.29	$1.10 \cdot 10^{-1}$
1	12.5	$1.02 \cdot 10^{-1}$	3.15	$1.07 \cdot 10^{-1}$	1.06	$1.13 \cdot 10^{-1}$	6.44	$1.12 \cdot 10^{-1}$	8.14	$1.10 \cdot 10^{-1}$
2	53.7	$9.69 \cdot 10^{-2}$	52.7	$9.97 \cdot 10^{-2}$	47.1	$1.12 \cdot 10^{-1}$	17.3	$1.12 \cdot 10^{-1}$	58.4	$1.10 \cdot 10^{-1}$
3	83.1	$7.61 \cdot 10^{-2}$	77.7	$7.59 \cdot 10^{-2}$	63.8	$1.06 \cdot 10^{-1}$	112.0	$6.49 \cdot 10^{-2}$	80.1	$1.10 \cdot 10^{-1}$
4	96.0	$6.36 \cdot 10^{-2}$	89.5	$6.62 \cdot 10^{-2}$	73.8	$9.97 \cdot 10^{-2}$	113.0	$6.39 \cdot 10^{-2}$	83.1	$1.08 \cdot 10^{-1}$
5	102.0	$6.23 \cdot 10^{-2}$	99.8	$6.41 \cdot 10^{-2}$	84.9	$9.31 \cdot 10^{-2}$	116.0	$5.86 \cdot 10^{-2}$	90.2	$8.01 \cdot 10^{-2}$
6	111.0	$5.68 \cdot 10^{-2}$	111.0	$6.12 \cdot 10^{-2}$	91.8	$7.91 \cdot 10^{-2}$	509.0	$1.55 \cdot 10^{-3}$	151.0	$2.18 \cdot 10^{-2}$
7	136.0	$3.52 \cdot 10^{-2}$	128.0	$4.10 \cdot 10^{-2}$	105.0	$7.53 \cdot 10^{-2}$	566.0	$1.26 \cdot 10^{-3}$	592.0	$1.26 \cdot 10^{-3}$
8	249.0	$6.58 \cdot 10^{-3}$	213.0	$9.52 \cdot 10^{-3}$	128.0	$4.50 \cdot 10^{-2}$	826.0	$1.08 \cdot 10^{-3}$	654.0	$1.07 \cdot 10^{-3}$
9	980.0	$6.64 \cdot 10^{-4}$	916.0	$6.49 \cdot 10^{-4}$	962.0	$6.38 \cdot 10^{-4}$	1180.0	$4.53 \cdot 10^{-4}$	844.0	$1.48 \cdot 10^{-4}$

The first column presents the point number. Then the values of the (h,k) point are presented where the subscript indicated the applied objective function described earlier in this chapter (deviation, squared, relative, quotient and distance respectively). From this table it can be seen that, though the curves look similar, both the h and the k-values differ quite a lot between the objective functions.

2.3.2 Fitting h(θ) and K(h)

The sample considered next is one from a loamy soil near Catsop in the south-eastern part of The Netherlands (Code Cat3_0-8B, nr. 809 in the Priapus database (Stolte et al., 2007)). The hydraulic conductivity fit and the fit of soil moisture retention curve will be called kh809 en pF809 in this chapter. The Mualem - Van Genuchten parameters for this sample can be obtained from the database as well. These parameters are calculated with the default settings of the computer program RETC (Van Genuchten et al., 1991). The curves obtained with RETC do not fit the data very well. Therefore this was an excellent example to read into Splop and see what fits would be generated by that program. The results for the soil-moisture retention curve are shown in Figure 2.6.

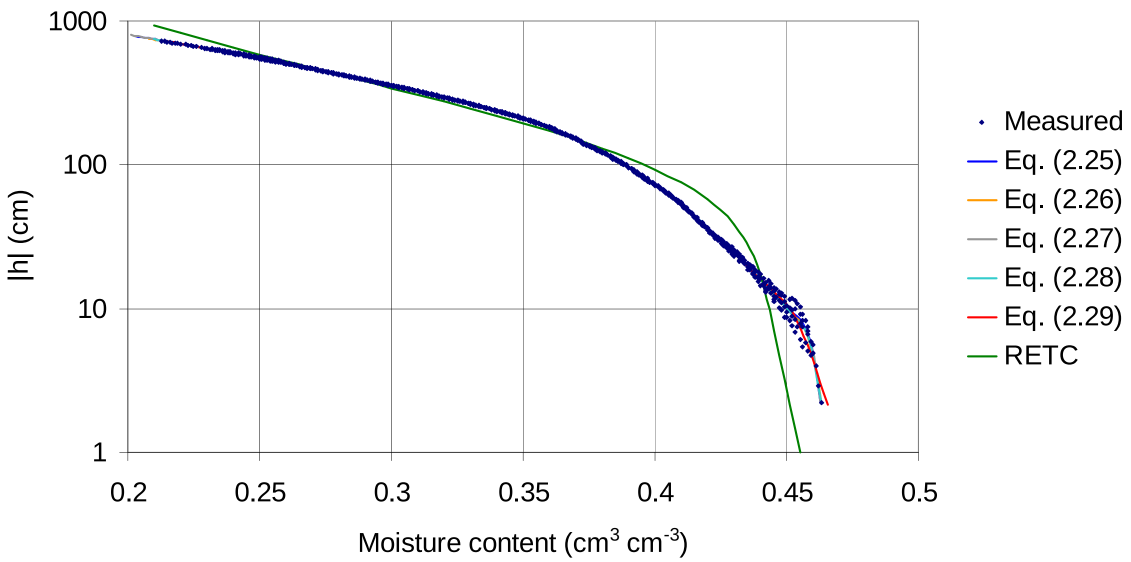


Figure 2.6 Measured and fitted relationships between pressure head h (cm) and moisture content θ ($cm^3 cm^{-3}$) for soil sample 809.

From this figure it can be seen again that all objective functions yield nearly the same result. Only at the wet side of the curve the 'distance' function shows a slight difference. This is caused by the fact that the lines are almost vertical here. On the other hand the difference with the results of RETC is considerable. This difference is probably caused by taking the measured hydraulic conductivities into account as well. These measured hydraulic conductivity values are shown in Figure 2.7, together with the computed results using the different objective functions.

Considerable differences exist between the results of the various objective functions due to the presence of only 2 points in the wet range, implying a lot of freedom in this zone. Again the objective function with the quotients is most divergent. As in the other example the values of 1 and -1 are yielding the same value of the objective function. In this figure the difference with the RETC-solution is even more pronounced than in the previous figure.

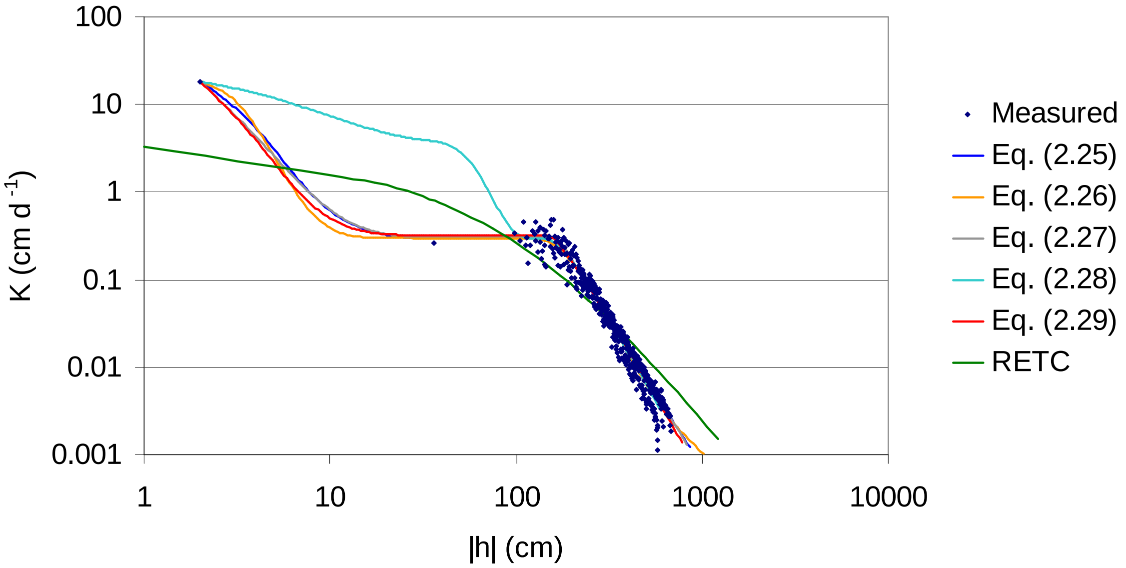


Figure 2.7 Measured and fitted relationships between hydraulic conductivity K (cm d^{-1}) and pressure head h (cm) for soil sample 809.

2.3.3 How many points are required?

In the optimizations described in the previous sections we assumed the spline-functions were described with 10 Virtual Data Points. To investigate the influence of the number of spline-points on the minimum value of the objective function, a number of optimizations were performed with different objective functions and different number of points. The data were taken from the Glanerbrug example again. The minimum value that was reached is presented in Table 2.2. Considering the decrease in the value of the objective functions when the number of points increases, it may be decided that 7 points is sufficient for the data presented here. This is just an indication. When the number of points increases beyond 8, the minimum reached does not significantly decrease, indicating that the introduction of more spline points will not yield a better fit, only additional computational efforts. The same conclusion can be found in literature (Bitterlich et al., 2004).

Table 2.2 Minima of objective functions g for different numbers of spline-points.

Points	Eq.(2.25)	Eq.(2.26)	Eq.(2.27)	Eq.(2.28)	Eq.(2.29)
3	105.17	26.55	82.25	20.80	24.06
4	96.34	18.44	72.34	12.93	21.75
5	88.26	16.09	65.10	12.08	19.51
6	88.22	16.00	64.70	11.70	19.47
7	87.96	15.49	65.07	11.45	19.47
8	87.90	15.49	64.78	11.44	19.12
9	87.86	15.48	64.63	11.44	19.10

2.3.4 The influence of the objective function

As was said before, the objective function with the squared deviation between measured and fitted values for a specified x (measured point) is most widely used. Intuitively however, the function that uses the distance between the (measured) point and the (calculated) line looks more reliable. Though at first sight all of the optimizations described in the previous sections yield good results, there are differences. These differences are hard to quantify however. One possible quantification is Mean Distance from Point to Line approach (MDPL, eq. (2.32)). This yields the function values in Table 2.3. It can be seen that the optimization procedure using the sum of distances as the objective function yields the best result and the RETC-fits yield the worse approximations. For the ’pF809’-case there are only slight differences between the objective functions. Here the order of accuracy is deviation, relative, quotient and squared.

Table 2.3 MDPL-values for the different optimization problems and with various objective functions.

Case	Eq. (2.25)	Eq.(2,26)	Eq, (2.27)	Eq. (2.28)	Eq. (2.29)	RETC
pF809	0.00257	0.00261	0.00256	0.00260	0.00246	0.02416
Kh809	0.01135	0.01152	0.01124	0.01298	0.01108	0.02967
Tox	0.00213	0.00213	0.00216	0.00218	0.00208	0.00446
hk61	0.02480	0.02481	0.02394	0.02375	0.02064	0.02743

For the kh809-data the relative deviation and the deviation method yield almost the same result as the distance-method. The value of the squared method is a little higher and the one of quotient is much larger. For the Tox data the order is deviation, squared, relative and quotient. In case of kh61, the deviation and squared method do yield nearly equal results. So do the relative and the quotient method. The relatively large difference between the distance and the other methods was already shown in Figure 2.3.

Figure 2.8 shows the percentages the MDPL is higher than the value obtained with the distance method for all other methods, as well as the average deviation. It can be seen that the deviations of the different spline approximations vary quite a bit. For the hk61-case all values are surprisingly high (15 - 20%). The deviations of the RETC-fits vary between 33% and 881%. The figure also shows the average deviation per object-function. These values are around 7%, except for the quotient method where it is 16% and 299% for RETC.

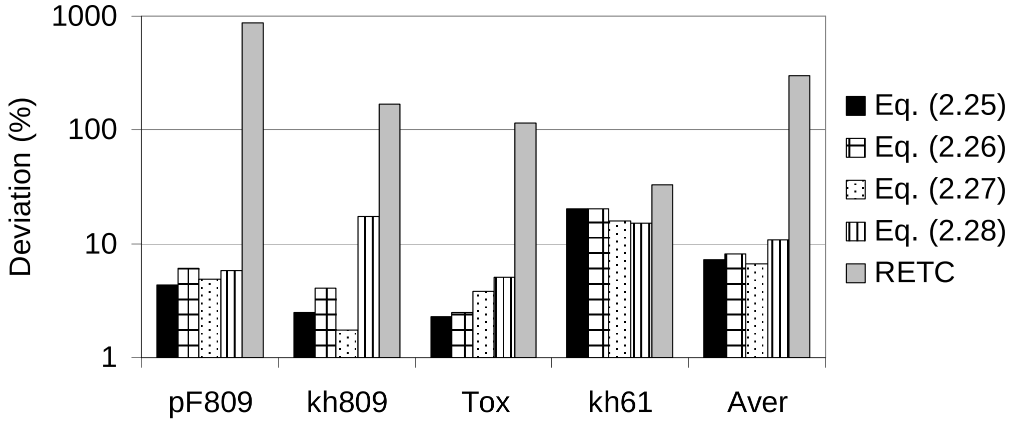


Figure 2.8 The deviation of the results of each optimization case and objective function from the one calculated with the sum of distances.

2.4 Conclusions

- Using either the Simplex or the CRS optimization procedure, the objective functions 'deviation', 'squared', 'relative' and 'distance' achieved satisfactory results for pF and K(h)-data. The 'quotient' function in its basic form did not satisfy our requirements. It yields excellent results as long as the y-values remain positive all the time. The best results were obtained with the ’distance’ objective function, however, this method requires more computer time.

- The spline approximation works very well to describe the soil physical relationships.
- The results of the different objective functions do yield differences in function values. They all yield some optimal curves, but the optima may differ from one another.
- The number of Virtual Data Points of a spline approximation is of some importance: if too few points are taken, the optimal value may not be approximated. If too many points are considered, there is no improvement of the optimal function compared to less points, in that case there is only an increase in computational efforts.
- The frequently used RETC fitting code can be improved by using the ’distance’ function instead of using the present ’squared’ objective function.

3 Soil physical classes: an evaluation of the Staring Series and directions for improvement

When simulating soil moisture flow with numerical models, information on the water retention characteristic and the (un)saturated hydraulic conductivity relation is required as input. In many cases these data are either not available or they are not representative for the soil horizon under consideration. Then one often uses some ‘averaged’ soil physical characteristics from an existing soil physical database. Frequently these characteristics are related to soil units with a certain texture and/or organic matter content. In this chapter the effects are investigated of taking these ‘averaged’ soil physical properties to compute steady-state and transient flow instead of using directly measured data belonging to this soil physical class. Results indicate that large differences might occur between using averaged soil physical properties versus directly measured data. More important, it became also clear that the way soil physical databases have been developed, for instance the well-known Staring Series, on basis of soil texture and organic matter differences, not necessarily result in significantly distinguishable soil physical classes. Better criteria are needed to group individual soil samples into unique soil physical classes.

Adapted from

Wesseling, J.G., C.J. Ritsema, K. Oostindie, L.W. Dekker, C.R. Stoof and H.R.J. Vroon. 2009. Soil physical classes: an evaluation of the Staring Series and directions for improvement. Submitted to Geoderma

3.1 Introduction

Due to the increasing capacity of computers, more and more numerical models for the simulation of both saturated and unsaturated soil moisture flow are being developed and applied. Most of these models are based upon the Richards' equation. This is a partial differential equation which requires the knowledge of two soil physical relationships: the soil moisture retention curve (the relationship between moisture content and pressure head) and the hydraulic conductivity curve (the relationship between hydraulic conductivity and pressure head). These relationships are strongly non-linear and different for each soil-layer. They are very important for obtaining an accurate description of unsaturated moisture flow and can be measured in the field or in the laboratory using different methods (e.g. Ahuja et al., 1980; Boels et al., 1978; Bouma and Denning, 1972; Bouma et al., 1971; Bresler et al., 1978; Kool and Parker, 1987a; Kool and Parker, 1987b; Stolte and Veerman, 1990; Van Dam et al., 1990b; Wind, 1966).

A description of the most commonly used methods to determine the unsaturated hydraulic conductivity of a soil has been presented by e.g. Dirksen (1990). A review of applied methods of calculating the unsaturated hydraulic conductivity from the degree of saturation has been presented by Brutsaert (1967). Sometimes the hydraulic conductivity function and the soil moisture retention curve are measured at the same time, e.g. by the evaporation method (Wind, 1966; Halbertsma and Veerman, 1994; Wendroth et al., 1993). One of the methods of estimating the hydraulic conductivity for high pressure heads (close to saturation) in the field is by means of infiltrometers (Logsdon and Jaynes, 1993). Rawls et al. (1991) presented a review of methods to obtain soil moisture retention curves from soil physical properties such as texture and bulk density.

In addition, several authors have tried to derive soil physical relationships from measured soil properties such as particle size distribution and organic matter content using pedotransfer functions (Ahuja et al., 1988; Alexander and Skaggs, 1987;

Bloemen, 1980; Bruce, 1972; Minasny and McBratney, 2007; Schuh and Bauder, 1986). These pedotransfer functions can be regarded as a bridge between pedology and hydrology and are gaining in popularity (Elsenbeer, 2001; Minasny et al., 1999; Nemes, 2003; Pachepsky et al., 2006; Rasiah and Aylmore, 1998; Wösten et al., 2001a). On the other hand, it has been shown also that pedotransfer functions developed on basis of sample characteristics obtained in certain sites or regions are not necessarily applicable in other areas (Li et al., 2007).

To derive continuous soil physical functions, fitting procedures are applied to measured data obtained in the laboratory or in the field. The quality of the fitted hydraulic properties strongly determines the reliability of flow and transport simulations. Many analytical equations have been developed to describe these relationships in a simple way, however, the most-widely used method is the one where the relationships are described by the Mualem-Van Genuchten equations (Van Genuchten, 1980). These equations describe both the soil moisture retention curve and the hydraulic characteristics with six parameters. Recently, Wesseling et al. (2008b) showed that fitting results can be improved by using a cubical spline method instead of the often used Mualem – Van Genuchten method.

During the last decade, soil physical properties have been brought together in soil physical databases like the Staring Series (Stolte et al., 2009; Wösten, 1987; Wösten et al., 2001b), the UNSODA database (Nemes et al., 2001) and the Hypres database (see http://www.macaulay.ac.uk/hypres/, Wösten et al., 1998). Some of these databases provide “average” soil physical properties for certain soil classes, meant for use in modeling studies and applications. The Staring Series present average soil physical properties for 36 different textural classes. Hypres contains both the “raw” measured data, parameters of the Mualem-Van Genuchten equations fitted through these raw data of individual samples and equations obtained with pedotransfer functions for 11 different textural classes. In UNSODA “raw” soil physical data is stored and 11 soil physical classes are distinguished.

The main objectives of this Chapter are i) to evaluate the performance of using such "averaged" soil physical properties compared to using measured data of individual samples and ii) to statistically analyse the hydrological differences between the soil physical classes of the Staring Series.

3.2 Theory

A number of analytical functions have been developed to describe the soil moisture retention and hydraulic conductivity relationships directly for individual samples without using the pedotransfer approach. Overviews and comparisons of different closed-form expressions can be found in the literature (e.g. Leij et al., 1997; Leong and Rahardjo, 1997).

One of the most frequently used closed-form expressions of the soil physical relationships is the one introduced by Van Genuchten (Van Genuchten, 1980) who describes the K(h)- and h(θ)-relationships as S-shaped curves with just six parameters:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\left(1 + |\alpha h|^n\right)^m} \tag{3.1}$$

$$h = \frac{\left(\left(\frac{\theta_s - \theta_r}{\theta - \theta_r}\right)^{\frac{1}{m}} - 1\right)^{\frac{1}{n}}}{\alpha} \tag{3.2}$$

$$K = K_0 \frac{\left(\left(1 + |\alpha h|^n\right)^m - |\alpha h|^{n-1}\right)^2}{\left(1 + |\alpha h|^n\right)^{m(l+2)}} \tag{3.3}$$

with

$$m = 1 - \frac{1}{n} \tag{3.4}$$

Differentiation of equation (3.2) with respect to h also yields an equation for the differential moisture capacity:

$$C_\theta = \frac{\partial \theta}{\partial h} = n \cdot m \cdot \alpha \cdot |\alpha h|^{n-1} \cdot \frac{\theta_s - \theta_r}{\left(1 + |\alpha h|^n\right)^{m+1}} \tag{3.5}$$

where h = pressure head (cm), θ = moisture content ($cm^3 cm^{-3}$), K = hydraulic conductivity (cm d^{-1}) and C = differential moisture capacity (cm^{-1}); α (>0, in cm^{-1}) is related to the inverse of the air entry suction; n (>1) is a measure of the pore-size distribution; K_0 is a fitted matching point at saturation (cm d^{-1}) and l is an empirical parameter that is normally assumed to be 0.5. The value of K_0 is often replaced by the saturated hydraulic conductivity K_s since K_s can be measured in a relatively simple way. K_0 is generally one order of magnitude lower than K_s (Schaap and Leij, 2000), and as such not really usable for model applications. Several improvements of this closed-form approximation have been proposed (Fuentes et al., 1992; Fuentes et al., 1991), especially near saturation (Schaap and van Genuchten, 2006; Vogel et al., 2001). Parameters for the closed-form expressions can be determined with several approaches. One of them is inverse modelling of soil moisture flow (Butters and Duchateau, 2002; Jhorar et al., 2001; Roulier and Jarvis, 2003; Sonnleitner et al., 2003; Yeh, 1986). In some publications the inverse modelling includes both solute transport and moisture flow (e.g. Abbasi et al., 2003). Methods have also been developed to estimate some of the Van Genuchten parameters taking into account their uncertainty (e.g. Abbaspour et al., 1997).

As mentioned before, both steady-state and transient soil moisture flow depends on the soil physical properties of the respective soil layers. Several methods have been applied to investigate the sensitivity of soil moisture flow to one or more soil physical parameters. Studies have been performed using numerical models (e.g. Sandhu, 2003; Simunek and van Genuchten, 1996). Other authors have applied a Monte-Carlo analysis for this purpose (e.g. Lu and Zhang, 2002; Mertens et al., 2005).

Most authors only perform a sensitivity analysis by varying just one or two parameters and evaluating the effect on model output (e.g. Hari Prasad et al., 2001). Rocha et al.

(2006) showed that calculations of subsurface flow in furrows was most sensitive to changes in n and in θ_s. A study by Lu and Zhang (2002) reported that n was the most sensitive parameter, followed by α and K_s.

To obtain the parameters of the Mualem-Van Genuchten equations from laboratory data, the curves should be fitted through a number of points. One of the most commonly used fitting programs is RETC (Van Genuchten et al., 1991), which is based upon the Marquardt-algorithm (Marquardt, 1963). Due to the strong non-linear form and the complexity of the Van Genuchten equations it is difficult to estimate the influence of each parameter on the soil moisture retention and hydraulic conductivity curves, and thus on the computed soil water content or pressure head. In the UNSODA database and the HYPRES database, samples are described using the Mualem - Van Genuchten parameter sets as fitted by RETC. The Staring Series only presents the parameters of the considered textural classes.

3.3 Materials and methods

3.3.1 The Staring Series

As an example, in this study we focus on two soil physical databases developed in The Netherlands: the Staring Series (Wösten, 1987; Wösten et al., 2001b), developed in the past, and Priapus (Stolte et al., 2007) which was developed recently. Over the last few decades a large number of soil samples has been analyzed in the soil physical laboratory of Alterra Wageningen, The Netherlands. In most cases, the soil physical properties (soil moisture retention curve and hydraulic conductivity relationship) were determined, as well as the soil texture and organic matter content. In first instance, these samples were used to create the Staring Series (Wösten, 1987; Wösten et al., 2001b), a dataset of soil hydraulical properties for Dutch soils. Eighteen different soil physical classes were distinguished for both topsoils and subsoils. Samples were grouped in these classes based upon information on texture and organic matter content (Table 3.1). The program RETC (Van Genuchten et al., 1991) was applied to determine the six parameters of the Mualem-Van Genuchten equations for each soil sample. With these six parameters, the soil moisture content and hydraulic conductivity were computed for a set of 13 specified pressure heads (-1, -10, -20, -31, -50, -100, -250, -500, -1000, -2500, -5000, -10000 and -16000 cm). Within each soil physical class the average value of hydraulic conductivity and moisture content were computed at each of the 13 pressure heads. Thereupon, a curve was fitted through these averaged 13 points of each relationship, yielding a set of six parameters for each soil physical class. As an example, Figure 3.1 shows the soil physical relationships of all the samples of class B8. The black line represents the average properties of this particular soil physical class. In the remainder of this Chapter these 'averaged' soil physical data will be referred to as the 'Staring data' as they are used in other studies most frequently. The soil physical characteristics per soil physical class were published and referred to in several reports (e.g. Wösten, 1987; Wösten et al., 2001b). Although these reports mention limitations of the possible application of these data, numerous calculations on the flow of both moisture and dissolved compounds were performed in The Netherlands using these derived properties (Massop et al., 2005; Massop et al., 2000; Wesseling et al., 2006; Wolf et al., 2003), amongst others leading to recommendations and governmental regulations regarding nutrient and pesticide use on agricultural land.

3.3.2 The Priapus database

More recently, an attempt has been made to recollect the original laboratory measurements of all individual soil samples that have been used to create the Staring Series. The data that has been found has been stored now in a database called Priapus. Data from more recently analyzed soils were added to the database also (Stolte et al., 2007; Stolte et al., 2009). In total 860 samples were added to Priapus, of which only 204 samples provided complete information on sampling location and depth, texture,

Table 3.1 The definition of the soil physical texture classes of the Staring Series with, if available, their ranges in percentages of clay, loam, organic matter and the median value of the particle size of the sand fraction, and number of soil samples (after Wösten et al., 2001b).

Class	Name	Clay (< 2 µm) %	Loam (2 - 50 µm) %	Org. matter %	M50 µm	Samples
Topsoils						
B1	Non-loamy sand		0-10	0-15	105-210	32
B2	Loamy sand		10-18	0-15	105-210	27
B3	Very loamy sand		18-33	0-15	105-210	14
B4	Extremely loamy sand		33-50	0-15	105-210	9
B5	Coarse sand			0-15	210-2000	26
B6	Boulder clay		0-50	0-15	50-2000	8
B7	Sandy loam	8-12		0-15		6
B8	Silt loam	12-18		0-15		43
B9	Clayey loam	18-25		0-15		29
B10	Light clay	25-35		0-15		12
B11	Heavy clay	35-50		0-15		13
B12	Very heavy clay	50-100		0-15		9
B13	Loam		50-85	0-15		10
B14	Heavy loam		85-100	0-15		67
B15	Peaty sand	0-8		15-25		10
B16	Sandy peat	0-8		25-100		20
B17	Peaty clay	8-100		16-45		25
B18	Clayey peat	8-100		25-70		20
Subsoils						
O1	Non-loamy sand		0-10	0-15	105-210	109
O2	Loamy sand		10-18	0-15	105-210	14
O3	Very loamy sand		18-33	0-15	105-210	23
O4	Extremely loamy sand		33-50	0-15	105-210	9
O5	Coarse sand			0-15	210-2000	17
O6	Boulder clay		0-50	0-15	50-2000	15
O7	River loam		33-50	0-15	50-150	15
O8	Sandy loam	8-12		0-15		14
O9	Silt loam	12-18		0-15		30
O10	Clayey loam	18-25		0-15		25
O11	Light clay	25-35		0-15		11
O12	Heavy clay	35-50		0-15		25
O13	Very heavy clay	50-100		0-15		19
O14	Loam		50-85	0-15		9
O15	Heavy loam		85-100	0-15		53
O16	Oligotrophic peat			35-100		16
O17	Eutrophic peat			35-100		36
O18	Peaty layer			15-35		7

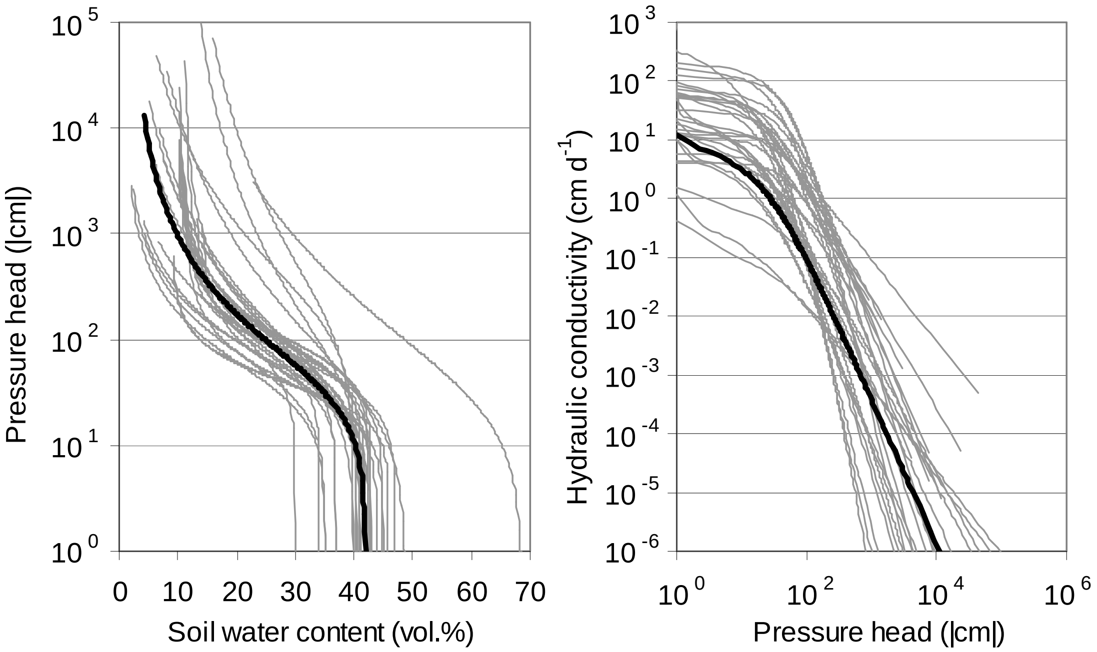


Figure 3.1. The soil moisture retention (left) and hydraulic conductivity (right) relations of the individual soil samples corresponding to Staring Series class B2. The black lines show the average relationships for class B2 as can be found in the Staring database (Wösten et al., 2001b)

organic matter content, dry bulk density, saturated hydraulic conductivity, raw data from the evaporation method, and fitted Mualem - Van Genuchten parameters. Each sample has been assigned again to one of the classes of the Staring Series based upon textural and organic matter information as done earlier also when constructing the Staring Series originally.

Table 3.2 presents the distribution of the soil samples over the original Staring Series soil classes together with the ranges of clay, silt and organic matter contents and the bulk densities. Unfortunately, eight classes of the Staring Series are currently not represented in Priapus because the original sample data got lost somehow. This concerns the classes B3, B14, O4, O5, O6, O7, O14 and O15.

An intranet application was created to make the database available for users within Alterra and Wageningen University at first instance. As the database contains samples from all over The Netherlands, it is the intention to make the Priapus database available for other users in and outside The Netherlands as well in a later stage, and to continuously update it whenever new samples are taken and determined in the laboratory.

3.3.3 Steady-state moisture flow

To evaluate the effects of using averaged soil physical properties instead of data from individual samples upon steady-state moisture flow, a simple program to compute steady-state situations for heterogeneous soil profiles was developed.

During the computations described in this Chapter, a flow domain consisting of a homogeneous soil profile with a fixed groundwater level at 150 cm depth has been considered. The program was applied to i) compute and visualize the pressure head profiles, and ii) find the maximum value of the flux that could reach the soil surface under steady-state conditions (i.e. the moisture flux at the top of the profile is kept constant until equilibrium is reached). These computations were performed for all 204 samples of the Priapus database in order to evaluate differences in soil hydrological behaviour between the samples, and between the different classes distinguished in the Staring Series.

3.3.4 Transient moisture flow

To investigate the differences in transient flow between different samples and classes, the numerical model SWAP (Van Dam et al., 1997a; 1997b) was applied. SWAP simulates transient moisture flow in a saturated/unsaturated 1-dimensional soil profile, and has been widely used in other studies also.

For this particular study, a homogenous soil profile, 1.5 m deep, was used, covered with grass. A set with measured daily precipitation and evaporation fluxes from the meteorological station of Wageningen University was applied to compute the moisture flux at the top boundary for the 40 year period of 1954-1993. The bottom boundary considered was free outflow, and no irrigation was applied. Maximum water

Table 3.2 The range of available soil textural data of the samples in the Priapus database grouped into the Staring Series classes. The last column (N_d) shows the number of soil samples in each class. Note that no information could be obtained for the classes B3, B13, B14. O4, O, O6, O7, O14 and O15.

Class	Name	<2 µm		2-50 µm		Org. Matter (%)		M50		Dry bulk density (g cm^{-3})		N_d
		Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	
Topsoils												
B1	Non-loamy sand			3.2	9.8	0.4	12.0	163	180	0.91	1.71	20
B2	Loamy sand			10.0	18.4	2.0	6.8	145	180	1.21	1.71	25
B4	Extremely loamy sand			17.7	28.0	6.0	9.9	135	163	1.17	1.52	8
B5	Coarse sand			5.0	12.4	0.3	3.3	56	282	1.30	1.50	11
B6	Boulder clay			24.8	43.6	0.9	2.5	350	505	1.51	1.64	4
B7	Sandy loam	8.5	10.2			1.6	11.1			0.88	1.62	7
B8	Silt loam	12.2	17.3			0.5	3.2			0.87	1.58	38
B9	Clayey loam	17.8	24.9			1.9	2.4			1.28	1.63	28
B10	Light clay	27.7	34.8			2.1	6.3			1.23	1.68	10
B11	Heavy clay	39.1	45.9			3.9	5.7			1.09	1.21	3
B12	Very heavy clay	51.4	82.9			2.9	12.1			0.89	1.35	31
B15	Peaty sand	2.6	2.6			6.4	18.6			0.96	0.96	1
B16	Sandy peat	5.1	5.1			30.0	31.2			0.56	0.56	1
B17	Peaty clay	8.0	61.2				31.7			0.48	0.97	8
B18	Clayey peat	52.4	80.1			39.2	61.7			0.38	0.62	6

Table 3.2 Continued

Class	Name	<2 µm		2-50 µm		Org. Matter (%)		M50		Dry bulk density (g cm^{-3})		N_d
		Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	
Subsoils												
O1	Non-loamy sand			2.8	8.1	0.1	2.3	117	190	1.50	1.80	16
O2	Loamy sand			10.2	14.5	6.2	4.4	123	175	1.45	1.77	3
O3	Very loamy sand			20.0	31.9	0.3	12.4	125	160	1.47	1.78	5
O8	Sandy loam	8.8	11.9			2.6	1.2			1.45	1.69	7
O9	Silt loam	12.2	17.4			0.4	13.0			0.74	1.69	16
O10	Clayey loam	18.0	22.8			0.2	6.3			1.09	1.55	7
O11	Light clay	25.0	30.0				4.8			0.96	1.45	6
O12	Heavy clay	37.2	46.7			4.7	13.7			0.78	1.33	8
O13	Very heavy clay	51.6	77.1			1.3	9.5			0.86	1.29	19
O16	Oligotrophic peat					0.1	96.3			0.11	0.19	4
O17	Eutrophic peat					82.2	81.8			0.14	0.39	10
O18	Peaty layer					38.3						7

ponding on the soil surface was set to 5 mm, additional water was considered to be surface runoff. Results were analyzed regarding terms of the overall water balance.

3.4 Results and discussion

3.4.1 Steady-state moisture flow

As an example, Figure 3.2 presents pressure head profiles for all 25 soil samples in soil physical class B2 of the Staring Series in case of 4 mm d^{-1} capillary rise and a groundwater level at 150 cm below the soil surface. The solid black line represents the pressure head profile computed with the parameters of the (averaged) B2 class of the Staring Series. Figure 3.2 clearly shows that capillary rise for only a few samples transports water up to the soil surface with the specified rate, other profiles barely yield a 20 cm capillary rise. This indicates that clustering of samples based on similar texture and organic matter classes not necessarily leads to comparable capillary behavior. A second characteristic compared is the maximum value of the soil moisture flux that is able to reach the surface under steady-state conditions for each sample in class B2 using a fixed groundwater level of 100 cm below the soil surface. The distribution of these maximum fluxes is presented in Figure 3.3. For 9 of the 25 samples the moisture flux could not reach the soil surface. These calculations were repeated for all samples of each of the Staring Series classes and for the averaged Staring data. The results are presented in Table 3.3, showing the median and average fluxes, amongst others. The median value is the flux-value whereby half of the considered values is lower. If the median value is lower than the average value, most of the samples show fluxes lower than the average value. This is exhibited for 20 of the 36 Staring Series classes.

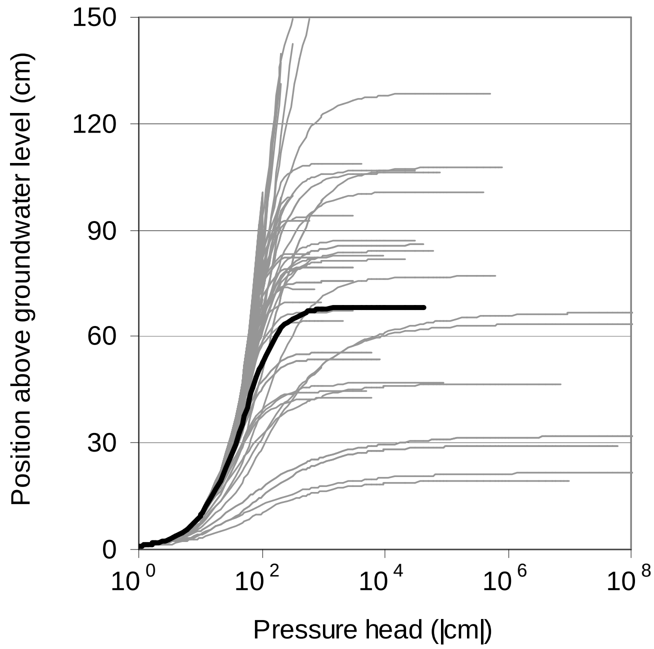


Figure 3.2 Computed pressure head profiles of the samples corresponding to the B2-class for a homogeneous 1.5 meter deep soil profile and an upward directed steady-state flux of 4 mm d^{-1}. The black line represents the profile computed with the average Staring relationships of class B2.

The columns Q_u show the maximum values computed with the averaged Staring data. The differences between the mean of the values calculated with the individual samples and the values computed with the averaged Staring data are considerable. The averaged flux-values of the individual samples and the fluxes from the Staring Series are presented in Figure 3.4. Note that the number of samples in each class (N_d) is lower in Table 3.3 than in Table 3.2 for some classes. This is due to the fact that both soil moisture retention curve and hydraulic conductivity functions were required to perform the calculations presented here.

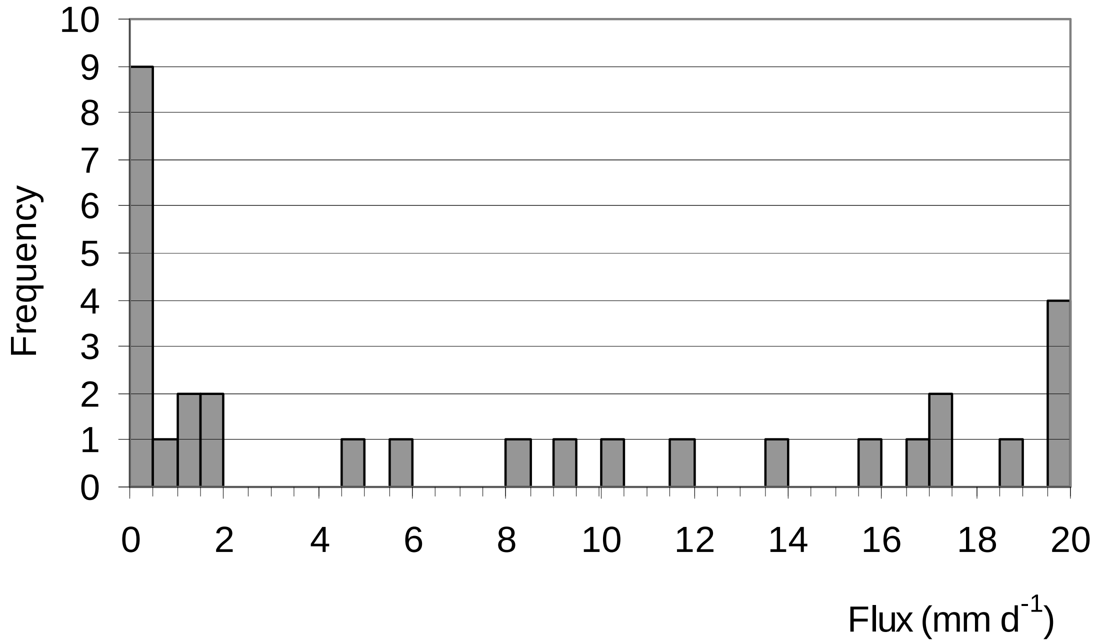


Figure 3.3 The distribution of the maximum values of the (steady-state) flux that reaches the soil surface for all samples of textural class B14 in case of a homogeneous soil profile and a groundwater level of 100 cm below soil surface.

3.4.2 Transient moisture flow

This section presents simulation results of transient moisture flow computations for individual samples and averaged Staring data for a 40 year period. Results presented focus on differences in plant evaporation ratio, soil evaporation, surface runoff and the flux through the bottom of the profile as averages of the annual values.

The computed average surface runoff amounts for all Staring Series classes are shown in Figure 3.5. Although these values are not specifically relevant in practice for the subsoil classes, they are presented here as well to indicate the variation between all classes. Variation in computed values of surface runoff is larger for topsoils than for subsoils. For the topsoils the largest variation is found for textural classes B12 and

Table 3.3 Fluxes (mm.d[-1]) for all samples in the different Staring Series classes that can, under stationary circumstances, reach the surface of a homogeneous soil profile with a groundwater level at 100 cm depth. N_d = number of samples, Min = minimum of calculated fluxes, Max = maximum of calculated fluxes, Median = median value of calculated fluxes, s.d. = standard deviation of fluxes, Mean= average value of calculated fluxes and Q_u is the maximum flux calculated with the averaged parameters as presented in the original Staring Series (Wösten et al., 2001b).

Class	N_d	Min	Mean	Max	Median	S.d.	Q_u	Class	N_d	Min	Mean	Max	Median	Std.dev.	Q_u
B1	14	0.19	2.09	5.69	1.11	1.97	2.02	O1	16	0.19	3.44	13.13	2.51	3.61	1.29
B2	21	0.44	19.25	83.69	11.06	21.12	1.78	O2	3	0.07	1.41	2.76	1.41	1.34	1.41
B3								O3	5	0.32	29.61	74.90	4.95	37.92	2.88
B4	8	1.29	15.24	57.08	3.37	23.28	7.03	O4							
B5	10	3.61	29.47	134.59	5.02	44.85	0.93	O5							
B6	4	0.07	0.90	2.27	0.62	1.01	12.89	O6							
B7	7	0.44	1.57	5.56	0.80	1.85	1.78	O7							
B8	37	0.19	3.26	16.43	1.17	4.13	1.90	O8	7	0.32	2.16	6.05	1.90	1.84	3.25
B9	28	0.19	1.05	3.49	0.80	0.82	2.63	O9	16	0.32	2.93	10.08	2.09	2.85	2.27
B10	9	0.07	0.42	1.17	0.19	0.44	0.93	O10	7	0.44	2.16	7.03	0.80	2.57	1.29
B11	2	0.07	0.07	0.07	0.07	0.00	0.44	O11	6	0.19	0.58	1.54	0.25	0.57	1.05
B12	18	0.07	0.11	0.32	0.07	0.09	0.19	O12	6	0.07	0.56	1.17	0.44	0.42	0.44
B13								O13	14	0.00	0.12	0.32	0.07	0.08	0.19
B14								O14							
B15	1	0.32	0.32	0.32	0.32	.	2.27	O15							
B16	1	3.25	3.25	3.25	3.25	.	2.27	O16	1	8.98	8.98	8.98	8.98	.	0.93
B17	4	0.07	0.35	0.80	0.25	0.32	0.32	O17	2	0.32	0.56	0.80	0.56	0.35	1.29
B18	6	0.07	0.23	0.68	0.13	0.24	0.56	O18							

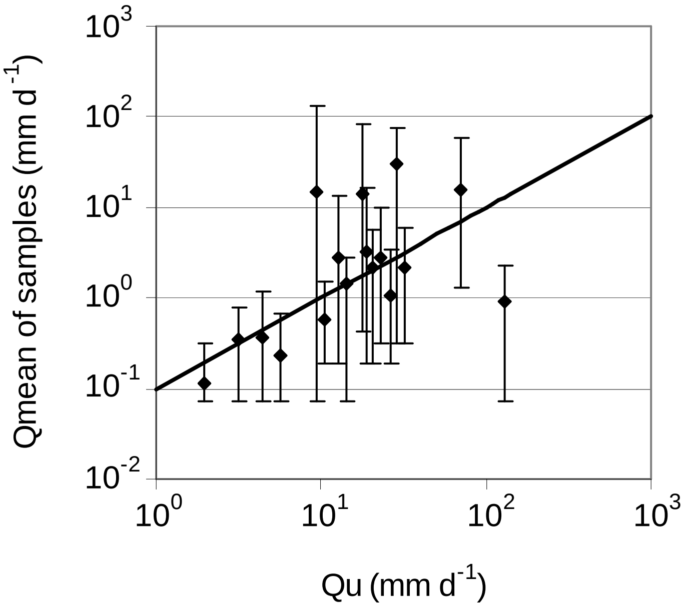


Figure 3.4 The maximum fluxes that reach the soil surface, assuming a groundwater level at 100 cm depth. Vertically the range of the maximum fluxes calculated with the individual samples are drawn together with the average value, horizontally the values obtained with the soil physical data of the corresponding Staring classes are presented.

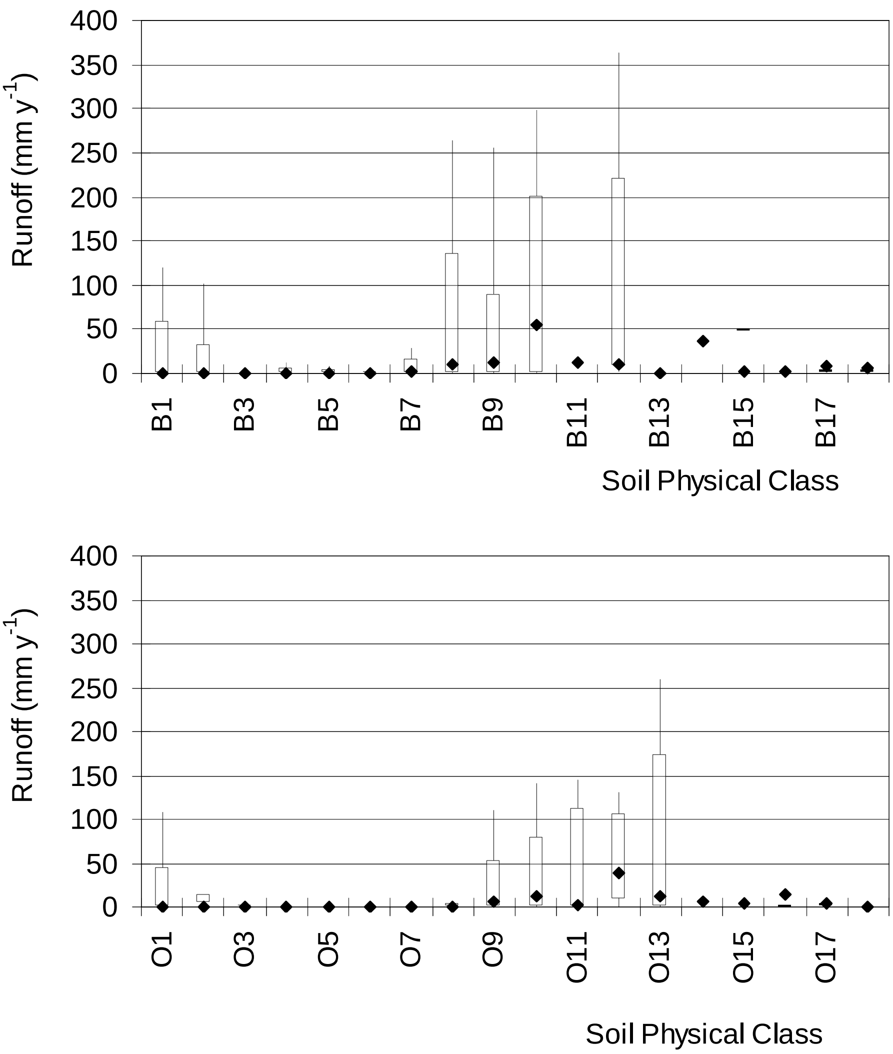
B10. For the subsoils the largest variations occur for the textural classes O13, O11 and O10. In general, runoff values obtained with the Staring data are on the (very) low side compared with the computed amounts for the individual samples.

A possible indicator for plant related soil moisture stress is the ratio between actual plant evaporation and potential plant evaporation. These ratios, averaged over the respective 40 year period, are presented in Figure 3.6. This figure shows a large range of values. The largest variation occurs for class B8: plant evaporation ratios range from 60 to 97%. The subsoils show a similar pattern as the topsoils do. In this case the largest differences occur for texture class O11: 69 to 86%. For both top and subsoils it is striking that in some cases (B5, B6, B10, B15, O8, O17) there is a large difference between the ratios obtained with the parameters of the separate samples and the ratio's obtained with the averaged Staring data. For others, the values obtained with the

Staring data fall within the range of the values obtained with the individual soil samples from the Priapus database. For the topsoils the results from the Staring data are generally higher than the results obtained with the individual samples, indicating that calculations with the averaged Staring data might potentially underestimate actual soil moisture stress.

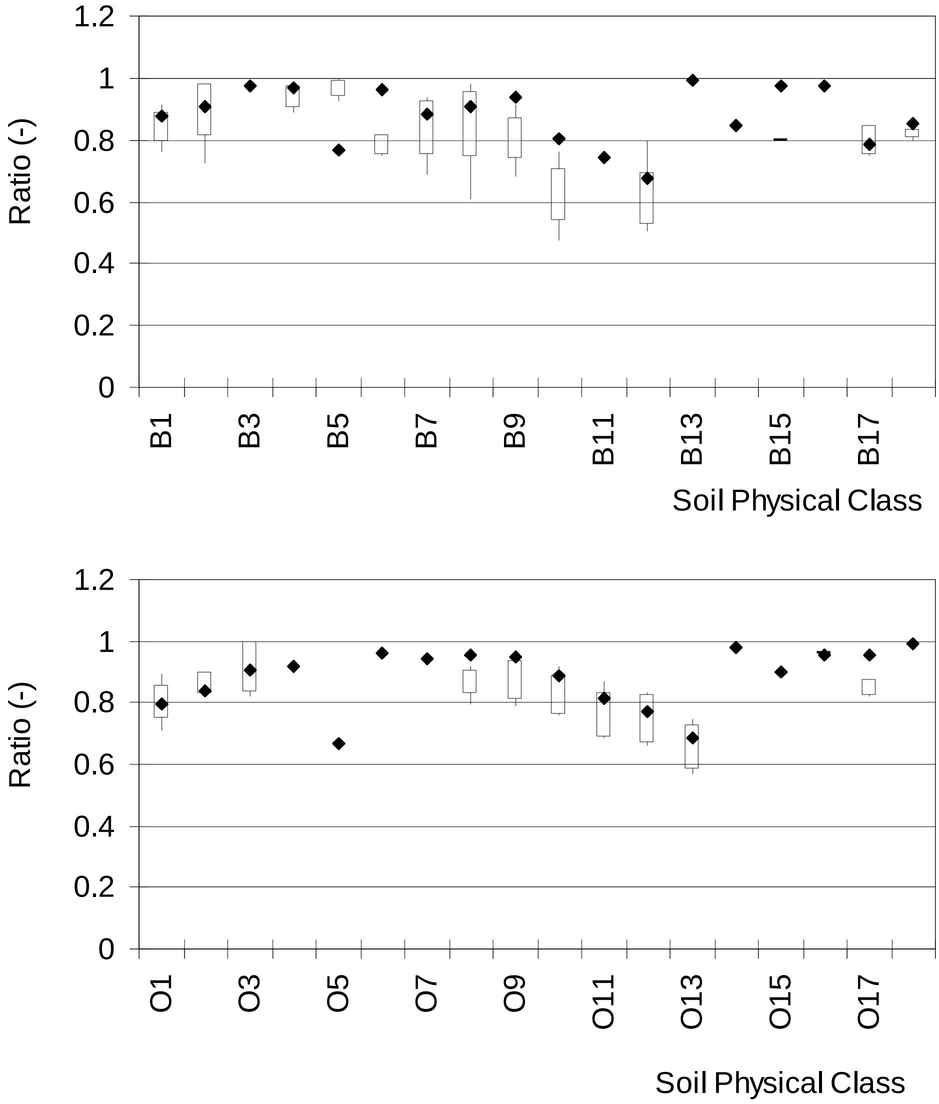
Also the actual soil evaporation rates appear to vary distinctly (Figure 3.7) between 72 and 102 mm y^{-1}. For a few soil physical classes the averaged Staring data results are lower than the ones calculated with the parameters of the individual samples. Nine values obtained with the averaged Staring data fall within the range of the values from the individual samples (B2, B4, B7, B10, B13, O1, O3, O11 and O13). The majority of the values obtained with the averaged Staring data is higher than the ones calculated on basis of the individual samples. For the samples of the subsoils approximately the same evaporation range can be observed as found for the topsoils. This basically means that by using averaged Staring data soil evaporation rates might be overestimated, at least for several of the Staring Series classes.

The majority of the values obtained with the averaged Staring data is higher than the range of soil evaporation values obtained with the individual soil samples from the Priapus database.



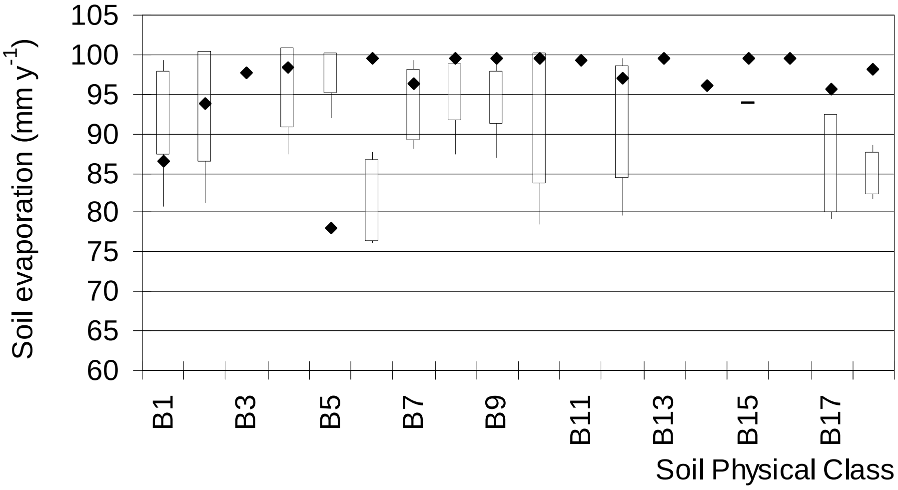
Soil Physical Class	Nr of Samples
B1	14
B2	21
B3	0
B4	8
B5	10
B6	4
B7	7
B8	37
B9	28
B10	9
B11	2
B12	18
B13	0
B14	0
B15	1
B16	1
B17	4
B18	6
O01	16
O02	3
O03	5
O04	0
O05	0
O06	0
O07	0
O08	7
O09	16
O10	7
O11	6
O12	6
O13	14
O14	0
O15	0
O16	1
O17	2
O18	0

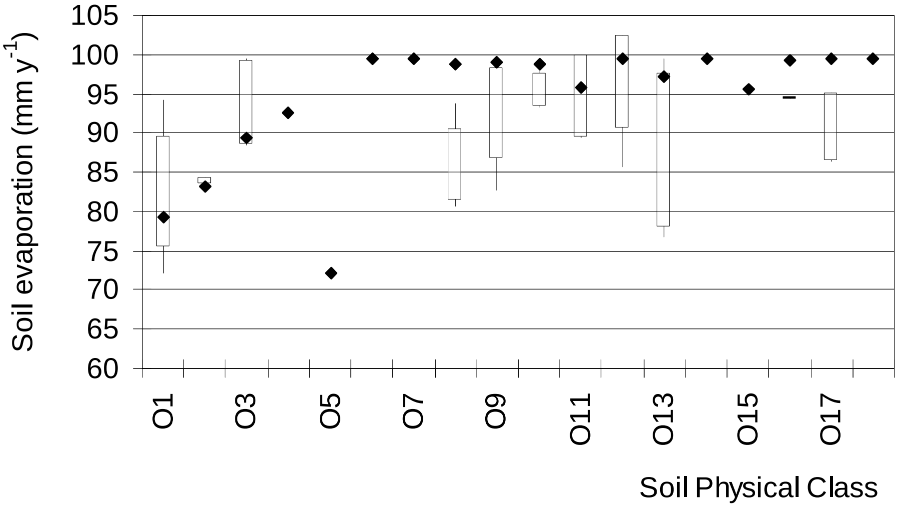
Figure 3.5 The yearly runoff rates for the individual soil samples as included in the Priapus database and assigned to the corresponding Staring Series classes. The endpoints of the thin lines represent minimum and maximum values, the top and bottom of the bar indicate the average + standard deviation and average – standard deviation. The diamonds indicate the values obtained with the averaged Staring Series data of the corresponding classes (Wösten et al., 2001b).



Soil Physical Class	Nr of Samples
B1	14
B2	21
B3	0
B4	8
B5	10
B6	4
B7	7
B8	37
B9	28
B10	9
B11	2
B12	18
B13	0
B14	0
B15	1
B16	1
B17	4
B18	6
O01	16
O02	3
O03	5
O04	0
O05	0
O06	0
O07	0
O08	7
O09	16
O10	7
O11	6
O12	6
O13	14
O14	0
O15	0
O16	1
O17	2
O18	0

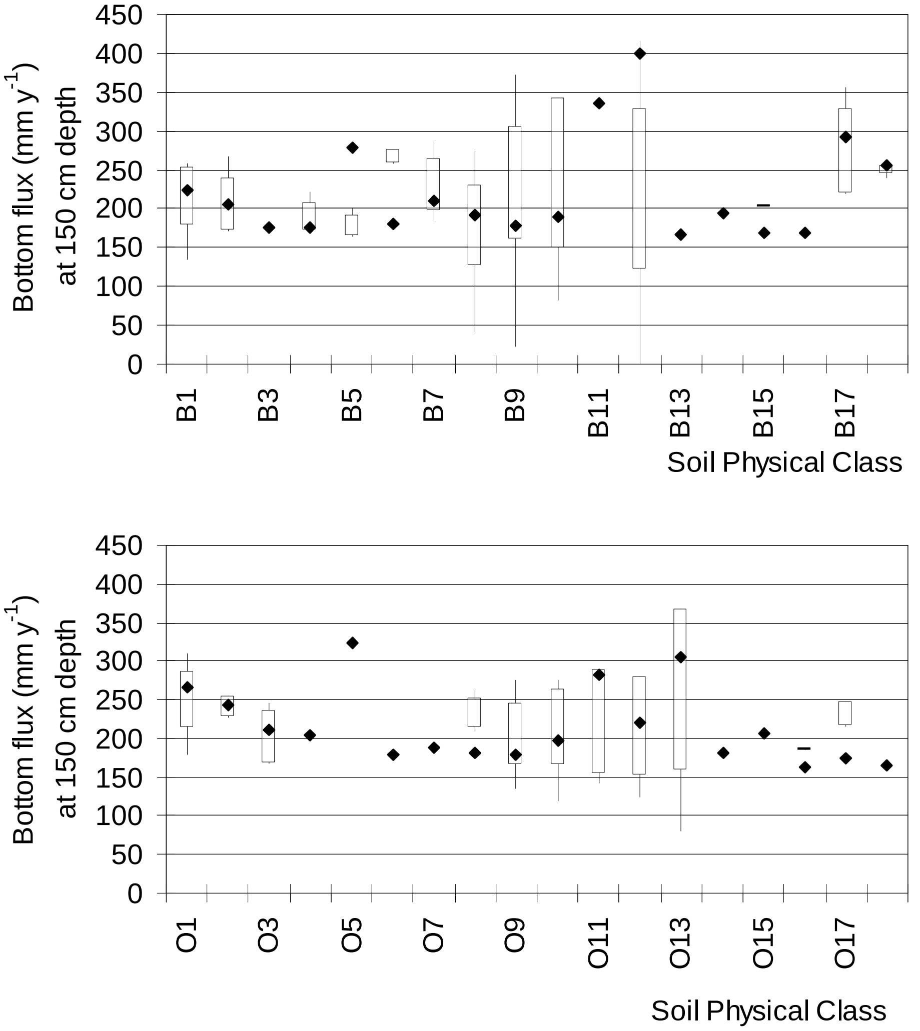
Figure 3.6 The ratios of actual and potential plant evaporation for the individual soil samples as included in the Priapus database and assigned to corresponding Staring Series classes. The endpoints of the thin lines represent minimum and maximum values, the top and bottom of the bar indicate the average + standard deviation and average – standard deviation. Diamonds are ratios obtained with the average Staring soil physical characteristics (Wösten et al., 2001b).





Soil Physical Class	Nr of Samples
B1	14
B2	21
B3	0
B4	8
B5	10
B6	4
B7	7
B8	37
B9	28
B10	9
B11	2
B12	18
B13	0
B14	0
B15	1
B16	1
B17	4
B18	6
O01	16
O02	3
O03	5
O04	0
O05	0
O06	0
O07	0
O08	7
O09	16
O10	7
O11	6
O12	6
O13	14
O14	0
O15	0
O16	1
O17	2
O18	0

Figure 3.7 The actual soil evaporation for the individual soil samples as included in the Priapus database and assigned to corresponding Staring Series classes. The endpoints of the thin lines represent minimum and maximum values, the top and bottom of the bar indicate the average + standard deviation and average – standard deviation. Diamonds are values obtained with the average Staring soil physical characteristics (Wösten et al., 2001b).



Soil Physical Class	Nr of Samples
B1	14
B2	21
B3	0
B4	8
B5	10
B6	4
B7	7
B8	37
B9	28
B10	9
B11	2
B12	18
B13	0
B14	0
B15	1
B16	1
B17	4
B18	6
O01	16
O02	3
O03	5
O04	0
O05	0
O06	0
O07	0
O08	7
O09	16
O10	7
O11	6
O12	6
O13	14
O14	0
O15	0
O16	1
O17	2
O18	0

Figure 3.8 The fluxes through the bottom of the soil profile for the individual soil samples as included in the Priapus database and assigned to the corresponding Staring Series classes. The endpoints of the thin lines represent minimum and maximum values, the top and bottom of the bar indicate the average +standard deviation and average – standard deviation. Diamonds are values obtained with the average Staring soil physical characteristics (Wösten et al., 2001b).

In regional studies in The Netherlands often the pesticide and nutrient loads to the surface- and groundwater are studied. Besides surface runoff, this load is calculated using the flux through the bottom of a 1-dimensional soil profile as well as the lateral flow components to the drains and ditches. The bottom fluxes obtained from our simulations with both the Staring data and the individual samples from the Priapus database are presented in Figure 3.8. The range of the bottom fluxes is large for some classes. The largest range is for B12: 0 to 416 mm y^{-1}. Classes B8, B9 and B10 show a large range as well. The largest variation in the bottom boundary fluxes for the subsoils is for class O13: 81 to 356 mm y^{-1}.

Computing the nutrient and pesticide loads with these percolation values may yield large differences! For the presented yearly fluxes through the bottom of the profile, the values obtained with the averaged Staring data generally fall within the range of the values obtained with the individual Priapus soil samples, except for the B12, O8 and O17 classes.

3.4.3 Statistical analysis

To test if there are significant hydrological differences between the (texture- and organic matter content based) classes of the Staring Series the results of the model simulations were statistically analyzed using SPSS (Version 15.0.1).

Due to the amount of classes and samples, the t-test could not be applied to check for any significant differences between the classes, and therefore the Bonferroni test was applied, which basically is a corrected t-test.

First it was tested whether the values of the saturated hydraulic conductivity showed a significant difference, as this is an input parameter for most numerical flow and transport models. It appeared there was no significant difference at all between the conductivities of any of the soil physical classes at a 0.05 level.

Furthermore, the computed surface runoff values were evaluated, as shown in Table 3.4. In this table (and the following ones), a ‘x’ indicates there is a significant difference (in this case in runoff amounts) (at a 0.05 level) between the values of the Staring Series class in the row and the values of the Staring Series classes in the different columns. Table 3.4 shows hardly any significant differences: only class B12 is significantly different from the other classes.

Also the plant evaporation ratios were statistically evaluated, as shown in Table 3.5. It clearly indicates that only the classes B10, B12 and O13 are significant different at the 0.05 level from most other classes. There are some individual differences (B5 is different from B8, B9, B10, B12, O1, O10, O11, O12 and O13), but in general the differences are not significant.

In Table 3.6 the results of the analysis of the actual soil evaporation are presented. Here only O1 differs significantly from most other classes. Compared to the transpiration ratio, this table shows considerably less x’s, so less signicant differences between the classes are present in this case.

Suprisingly, the values of the moisture flux through the bottom of the soil profile did not show any significant difference between the different classes of the Staring Series.

The previous tables clearly show that classifying soil samples in different categories on basis of soil texture and organic matter content alone as done previously in the Staring Series does not necessarily result in significant differences in hydrological behaviour. It appeared also that little differences exist between the original topsoil and subsoil classes of the Staring Series.

3.5 Conclusions

- Grouping soil samples into soil physical classes based upon texture and organic matter content alone as done earlier in the Staring database, does not yield satisfying results. Based upon hydrological computations, it has been shown that no significant differences occur between many of the original Staring Series classes. Better criteria are needed to group individual soil samples into unique (significantly different) soil physical classes.

- Use of "averaged" soil water retention and hydraulic conductivity curves as presented earlier in the Staring database (Wösten, 1987; Wösten et al., 2001b) might lead to deviations in computed moisture flow and transport compared to results obtained on basis of individual soil samples.
- It is recommended here to step away from the use of the original average Staring Series functions and to use soil physical characteristics of individual measured samples instead. Therefore soil physical characteristics should be measured more frequently in future studies and made accessible in databases for others as well.
- When adding new samples to a database such as Priapus, care should be taken that not only the measured soil physical data is reliable, but it should also have the appropriate metadata associated with it, like coordinates of the sampling position, sampling depth, type of soil, land use, laboratory method used, etc.

Table 3.4 Differences between the runoff values for the different soil physical classes of the Staring Series. A x means there is a significant difference at the 0.05 level.

Runoff	B1	B2	B4	B5	B6	B7	B8	B9	B10	B12	B17	B18	O1	O2	O3	O8	O9	O10	O11	O12	O13	O17	
B1																							B1
B2										x													B2
B4										x													B4
B5										x													B5
B6																							B6
B7																							B7
B8																							B8
B9										x													B9
B10																							B10
B12		x	x	x				x					x			x	x						B12
B17																							B17
B18																							B18
O1										x													O1
O2																							O2
O3																							O3
O8										x													O8
O9										x													O9
O10																							O10
O11																							O11
O12																							O12
O13																							O13
O17																							O17
	B1	B2	B4	B5	B6	B7	B8	B9	B10	B12	B17	B18	O1	O2	O3	O8	O9	O10	O11	O12	O13	O17	

Table 3.5 Differences between the plant evaporation ratios for the different soil classes of the Staring Sseries. A x means there is a significant difference at the 0.05 level.

Epa/Epp	B1	B2	B4	B5	B6	B7	B8	B9	B10	B12	B17	B18	O1	O2	O3	O8	O9	O10	O11	O12	O13	O17	
B1									x	x											x		B1
B2									x	x										X	x		B2
B4								x	x	x			x						x	X	x		B4
B5							x	x	x	x			x					x	x	X	x		B5
B6																							B6
B7									x	x											x		B7
B8				x					x	x											x		B8
B9			x	x					x	x											x		B9
B10	x	x	x	x		x	x	x			x	x	x	x	x	x	x	x				x	B10
B12	x	x	x	x		x	x	x			x	x	x	x	x	x	x	x				x	B12
B17									x	x													B17
B18									x	x													B18
O1			x	x					x	x											x		O1
O2									x	x													O2
O3									x	x											x		O3
O8									x	x											x		O8
O9									x	x											x		O9
O10				x					x	x											x		O10
O11			x	x																			O11
O12		x	x	x																			O12
O13	x	x	x	x		x	x	x					x		x	x	x	x					O13
O17									x	x													O17
	B1	B2	B4	B5	B6	B7	B8	B9	B10	B12	B17	B18	O1	O2	O3	O8	O9	O10	O11	O12	O13	O17	

Table 3.6 Differences between the actual soil evaporation values for the different soil classes of the Staring Series. A x means there is a significant difference at the 0.05 level.

Esa	B1	B2	B4	B5	B6	B7	B8	B9	B10	B12	B17	B18	O1	O2	O3	O8	O9	O10	O11	O12	O13	O17	
B1													x										B1
B2													x										B2
B4					x								x										B4
B5					x							x	x			x					x		B5
B6			x	x			x	x															B6
B7													x										B7
B8					x							x	x			x							B8
B9					x								x										B9
B10																							B10
B12																							B12
B17																							B17
B18				x			x																B18
O1	x	x	x	x		x	x	x							x		x	x		x			O1
O2																							O2
O3													x										O3
O8				x			x																O8
O9													x										O9
O10													x										O10
O11																							O11
O12													x										O12
O13				x																			O13
O17																							O17
	B1	B2	B4	B5	B6	B7	B8	B9	B10	B12	B17	B18	O1	O2	O3	O8	O9	O10	O11	O12	O13	O17	

4 A new, flexible and widely applicable software package for the simulation of one-dimensional moisture flow: SoWaM

Most one-dimensional soil moisture flow simulation models have restricted applicability due to (amongst other things): i) insufficient flexibility for the model users, ii) a lack of user friendliness, iii) only usable for certain spatial or temporal scales, and iv) fixed boundary conditions. Therefore, we developed a simple and highly flexible software package to simulate, visualize and analyze 1-D moisture flow in soils: SoWaM (Soil Water Model). The package has a modular setup and consists of a range of tools to visualize, analyze and compare input data and results. The governing Richards' equation is solved numerically by a time-centered Galerkin Finite Element approximation. Soil hydraulic properties for each specified soil layer can be defined by either Mualem - Van Genuchten parameters or splines. Since the model does not impose limits on element size or time interval, it is possible to perform simulations in very high detail, both spatially and temporally. Event-based precipitation as well as potential evapotranspiration are read from a database, in which the user can also specify the bottom boundary conditions. As opposed to most existing models, all (boundary) conditions in SoWaM are user-defined. This allows easy evaluation of the effects of different boundary conditions with regard to all terms of the water balance. Furthermore, four different criteria for irrigation scheduling have been implemented. The SoWaM package provides an accurate, simple and highly flexible tool to simulate soil moisture flow and to evaluate the effects of various factors on soil water movement, such as timing and amount of irrigation, soil hydraulic properties and soil layering.

Adapted from

Wesseling, J.G. , C.J. Ritsema, K. Oostindie, C.R. Stoof and L.W. Dekker. 2009. A new, flexible and widely applicable software package for the simulation of one-dimensional moisture flow: SoWaM. Submitted to Environmental Software and Modelling

4.1 Introduction

During the past decades numerical models for (one-dimensional) soil moisture flow have been developed all over the world, amongst others in Denmark (Hansen et al., 1990), France (Perrier et al., 2002), the United States (Simunek et al., 1998) and The Netherlands (Van Dam et al., 1997b). Recently, the Journal of Environmental Software and Modeling published a review of soil water numerical models that were developed and applied in Australia (Ranatunga et al., 2008). Those authors distinguished three different types of models: simple tipping-bucket models, layers tipping-bucket models and complex models. Generally, the complex models are based upon a (partial) differential equation like Richards' equation (Richards, 1931) which is solved numerically. A few of the numerical schemes include the finite difference method (Feddes et al., 1978; Freeze, 1971; Van Dam et al., 1997b; Watson et al., 1992), the integrated finite difference method (Hanks, 1991; Narasimhan et al., 1978), the Galerkin finite element method (Huyakorn et al., 1984), the collocation finite element method (Pinder et al., 1978), the subdomain finite element method (Cooley, 1983) and the spectral elements method (Goblet and Cordier, 1993). The methods applied by the authors mentioned above essentially differ with respect to spatial discretization and interpolation. Many additional features are available in some of these models, such as heat transport, solute transport, effects of frost, simple and detailed crop growth models, and others.

To simulate flow in high spatial and temporal resolution in structurally rigid porous media, either covered by vegetation or bare, a model is needed that is capable of computing one-dimensional water flow with i) high accuracy, ii) the ability to describe soil physical relationships in different ways, iii) the use of extremely small time intervals, iv) the ability of storing model output efficiently, and v) the ability to present output graphically. As none of the models found in the literature fulfilled all these requirements, the new SoWaM (Soil Water Model) software package was developed. In this chapter the model structure and its main properties are described, including some of the tools to create input and to analyze output. Furthermore, to illustrate model performance, two case-studies in which the model was applied are presented and discussed in Chapter 5 and Chapter 6 respectively.

4.2 Theory of soil moisture flow

4.2.1 The governing equations

Soil moisture flow in a 1-dimensional system can be described by the following partial differential equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K \frac{\partial H}{\partial z}\right) - S \qquad (4.1)$$

where H = total head [L]; z = coordinate in vertical direction [L]; θ = volumetric moisture content [L^3L^{-3}]; t = time [T]; K = prevailing hydraulic conductivity [LT^{-1}]; S = sink term representing drainage or root extraction [T^{-1}].

The total head H can be divided into two terms:

$$H = h + z \qquad (4.2)$$

where h = pressure head [L].

Introducing the differential moisture capacity C [L^{-1}] then yields

$$C \frac{\partial H}{\partial t} = \frac{\partial}{\partial z}\left(K \frac{\partial H}{\partial z}\right) - S \qquad (4.3)$$

with

$$C = \frac{\partial \theta}{\partial H} = \frac{\partial \theta}{\partial h} \qquad (4.4)$$

Both K and C-values depend on the prevailing pressure head h. To solve the partial differential equation, the C(h), K(h) and h(θ) relationships should be known. Equation (4.3) is known as the Richards' equation. This equation is also used in most other moisture flow models like Ecoul (Perrier et al., 2002), SWAP (Van Dam et al., 1997b), DAISY (Hansen et al., 1990) and Hydrus1d (Simunek et al., 1998).

4.2.2 Analytical approximation of soil moisture retention and hydraulic conductivity functions

The relationships between moisture content, pressure head and hydraulic conductivity are essential for a correct description of unsaturated moisture flow. These relationships can be measured in the field or in the laboratory using different methods (Ahuja et al., 1988; Bouma and Denning, 1972; Bresler et al., 1978; Kool and Parker, 1987a; Kool et al., 1987; Van Dam et al., 1990). Several authors have tried to derive these relationships by using pedotransfer functions and other known soil physical data, such as particle size distribution, texture and organic matter content (Ahuja et al., 1988; Alexander and Skaggs, 1987; Bloemen, 1980; Bruce, 1972; Schuh and Bauder, 1986; Wösten et al., 2001a). Although these pedotransfer functions are sometimes regarded as the bridge between pedology and hydrology and are gaining in popularity (Elsenbeer, 2001; Minasny et al., 1999; Nemes, 2003; Pachepsky et al., 2006; Schaap and Leij, 1998; Schaap et al., 2001; Stolte et al., 1996; Van Alphen et al., 2001), it has been shown that pedotransfer functions developed for one area do not always yield acceptable results in other areas (Li et al., 2007).

Several analytical functions have been developed to describe the soil moisture retention curve and/or the hydraulic conductivity relationship of a soil layer based on laboratory measurements. Overviews and comparisons of closed-form expressions can be found in the literature (e.g. Leij et al., 1997; Leong and Rahardjo, 1997). Nowadays the most frequently used closed-form description of soil physical relationships is the one introduced by Van Genuchten (Van Genuchten, 1980), who describes the $K(h)$- and $h(\theta)$-relationships as S-shaped curves with six parameters. Several improvements of this closed-form approximation have been proposed (e.g. Fuentes et al., 1992; Fuentes et al., 1991), especially near saturation (Schaap and van Genuchten, 2006; Vogel et al., 2001). The Mualem – Van Genuchten equations state

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\left(1 + |\alpha h|^n\right)^m} \tag{4.5}$$

$$h = \frac{\left(\left(\frac{\theta_s - \theta_r}{\theta - \theta_r}\right)^{\frac{1}{m}} - 1\right)^{\frac{1}{n}}}{\alpha} \tag{4.6}$$

$$K = K_0 \frac{\left(\left(1 + |\alpha h|^n\right)^m - |\alpha h|^{n-1}\right)^2}{\left(1 + |\alpha h|^n\right)^{m(l+2)}} \tag{4.7}$$

with

$$m = 1 - \frac{1}{n} \tag{4.8}$$

Differentiation also yields an equation for the differential moisture capacity:

$$C_\theta = \frac{\partial \theta}{\partial h} = n \cdot m \cdot \alpha \cdot |\alpha h|^{n-1} \cdot \frac{\theta_s - \theta_r}{\left(1 + |\alpha h|^n\right)^{m+1}} \tag{4.9}$$

where h = pressure head [L] (cm), θ = moisture content [L^3L^{-3}] ($cm^3\ cm^{-3}$), K = hydraulic conductivity [LT^{-1}] (cm d^{-1}), C = differential moisture capacity [L^{-1}] (cm^{-1}), α [L^{-1}] (>0, cm^{-1}) is related to the inverse of the air entry suction, n (>1) is a measure of the pore-size distribution; K_0 [LT^{-1}] is a fitted matching point at saturation (cm d^{-1}) and l is a dimensionless empirical parameter.

In some cases the parameters for the closed-form expressions can be determined by inverse modeling of soil moisture flow (Abbasi et al., 2003; Dahiya et al., 2007; Jhorar et al., 2001; Roulier and Jarvis, 2003; Sonnleitner et al., 2003; Yeh, 1986), but most of the time the parameters are still derived using laboratory data.

The main advantage of the Mualem - Van Genuchten equations is their simplicity. Six parameters are required to describe both the soil moisture retention curve and the hydraulic conductivity function. At the same time this is also the main disadvantage because sometimes relatively poor fits of the functions through the measured data are obtained. Instead of using a closed-form description of the soil physical relationships, some numerical models use soil physical characteristics described by tables with data-pairs, i.e. volumetric moisture content with pressure head (θ,h) and pressure head with hydraulic conductivity (h,K)-points. To obtain the corresponding values between the specified points, linear interpolation is applied (sometimes on a logarithmic scale). This can cause unnecessary iterations: the differential moisture capacity (the first derivative of the (continuous) soil moisture retention curve) is discontinuous, which causes ‘jumps’ between the values on the left hand and right hand side of a point. To ensure continuity of a function and its derivatives, splines can be used. This is one of the most powerful mathematical methods to describe a function. Splines are piecewise-continuous polynomials. Several types of splines have been applied in soil science, such as cubic splines (Hampton, 1990; Kastanek and Nielsen, 2001; Prunty and Casey, 2002; Wesseling et al., 2008b) and quadratic B-splines (Bitterlich et al., 2004). In the SoWaM package, both the cubic spline interpolation approach (Wesseling et al., 2008b) and the Mualem - Van Genuchten equations (Van Genuchten, 1980) have been incorporated to describe the physical properties of a soil layer.

4.3 Description of the software package

4.3.1 General

To solve the general equations described in the previous sections, the software package SoWaM was developed. It is applicable to all kinds of field situations, both agricultural and non-agricultural. The package consists of a number of modules: a basic SoWaM package and several supplemental modules/tools. The basic package includes a MySQL database (SoWaMData) and a program to simulate one-dimensional moisture flow (SoWaMCalc). The module SoWaMVis was developed to visualize, analyze and compare the results of the simulations. The soil physical properties of soil layers can be visualized with the module SoWaMSoil. A series of cubical splines can be fitted through a set of measured data with the module

SoWaMFit, and SoWaMDrain can be applied to determine the relationship between the groundwater level and the drainage flux. These latter two programs store their results directly into the database SoWaMData (Figure 4.1).

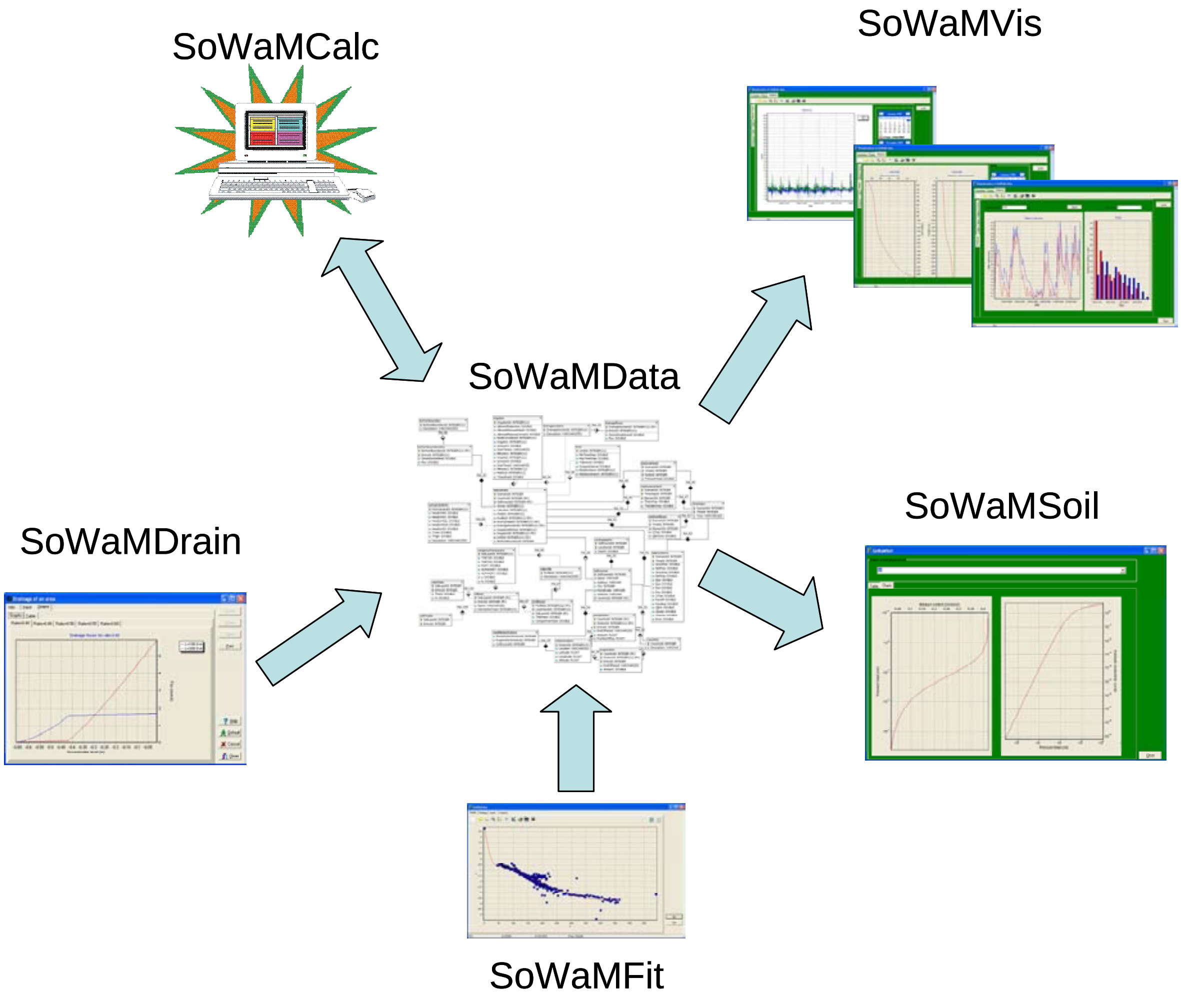


Figure 4.1 The components of the SoWaM software package.

4.3.2 SoWaMData

Nowadays most simulation programs read their input from a text file and store the results of simulations in another text file, either directly or through some kind of Graphical User Interface. The advantages of writing the output to a text file are that one can view the file with a regular text editor and that it can be printed directly or used as input for postprocessing programs. The disadvantage, however, is that these files need to be stored somewhere, which requires (possibly complex) data administration. Since we expected to perform many runs and to generate much input and output data, it was decided to store the input and output in a database using MySQL (see www.MySQL.org) with phpMyAdmin (www.phpMyAdmin.net) as its control system. These programs are open source software and can be downloaded free of charge. The database consists of 27 tables for input and 6 tables for output. It is beyond the scope of this Chapter to discuss the database in further detail.

4.3.3 SoWaMCalc module

4.3.3.1 General

The equations described in the theory-section of this Chapter have been solved using the Galerkin Finite Element Method. The program was tested by comparing the results of simulations with the results of analytical solutions (where available) and with the results of other programs such as SWAP (Kroes and van Dam, 2003; Kroes et al., 2008; Van Dam et al., 2008). Because results obtained with SoWaMCalc were similar to the ones obtained by SWAP, they are not presented in this Chapter.

4.3.3.2 Soil physical relationships

The program requires soil physical relations for each layer distinguished in the soil. These relationships can be described either with the parameters of the Mualem - Van Genuchten equations (Van Genuchten, 1980) or by the virtual nodes of spline functions (Wesseling et al., 2008b). It is also possible to have a combination of these, e.g. the top layer is described by the Van Genuchten equations and the sub layer(s) are presented with the spline-approximation.

4.3.3.3 Discretization

To solve the general flow equations, the soil profile is discretisized into a number of elements. Each element is bounded by one node at the top and one node at the bottom. In these nodes the pressure head and moisture content values are computed. The discretization is performed by the program itself. The user only has to specify the required element size in a specified zone, e.g. elements with size 0.1 cm in the zone until 0.5 cm depth. It is recommended that the smallest elements will be created where the largest gradients are expected.

4.3.3.4 Top boundary

To compute moisture flow in the soil profile, the database requires an amount of precipitation (P, mm) and potential evapotranspiration (E_t^p, mm) over a certain time period, including the start and end date and time. Precipitation data from automatic rain gauges can be entered directly into the database without the need for aggregation to obtain daily values (and thus loss of information). The program then computes the precipitation rate from the amount of precipitation and the time-period between entries. The same is done for the potential evapotranspiration data, yielding distributions of both precipitation and evaporation in time, respectively.

The potential evapotranspiration (E_t^p) is divided into potential soil evaporation (E_s^p) and potential plant evaporation (E_p^p) by the following equation:

$$E_s^p = E_t^p \cdot e^{-f \cdot LAI} \qquad (4.10)$$

where f is an empirical factor (dimensionless) and LAI is the Leaf Area Index (m^2m^{-2}) (Belmans et al., 1983; Goudriaan, 1977; Van Dam et al., 1997b).

4.3.3.5 Root water uptake

In the present version of SoWaM the rooting depth is considered to be constant. Roots are assumed to be distributed homogeneously throughout the rootzone. The uptake of water by plants depends on the prevailing pressure head. If the pressure head is too high (wet conditions), plants will suffer stress because the roots can not take up sufficient oxygen. If the pressure head is too low (dry conditions), plants will suffer as well because the energy required to extract the water from the soil matrix can not be supplied. In both cases root water uptake is far from optimal:

$$U_r^a(z) = U_r^p(z) \cdot g(h) \qquad (4.11)$$

where U_r^p and U_r^a are the potential and actual root water uptake per unit of length [T^{-1}] and g(h) is a factor between 0 and 1, depending on the pressure head h (Feddes et al., 1978; Van Dam et al., 1997b). The function value g represents a multiplication factor to obtain the actual plant evaporation from the potential plant evaporation. In case of grass, optimal water uptake (g=1) occurs when the pressure head is between -200 and -25 cm (Taylor and Ashcroft, 1972; Van Dam et al., 1997b). If the pressure head is outside this range, a reduction in plant evaporation will take place (g < 1). The actual plant evaporation (E_a^p) can be calculated according to

$$E_p^a = \int_{z_r}^{0} U_r^a(z)dz = \int_{z_r}^{0} U_r^p(z)g(h)dz \tag{4.12}$$

where z_r [L] is the bottom of the root zone. The pressure head values for the root uptake function are supplied by the user and read from the database.

4.3.3.6 Drainage

In many situations subsurface drainage will take place through furrows, drainpipes or ditches. In these cases the relationship between the groundwater depth and the magnitude of the flow to the drains has to be known. SoWaM requires this relationship to be entered as a number of points. The exact flux to the drainage media is obtained by linear interpolation between these specified points. An example of such a relationship is presented in Figure 4.2. In this figure, three drainage systems are assumed to be involved: a primary open system (canal) with a bottom depth of -1.6 m, a secondary open system (ditch) at -1.2 m and pipe drains at -0.4 m. As long as the groundwater level is below the bottom of the lowest drainage medium (-1.6 m), no water will flow to any drainage medium. If the water level rises above that level, water will flow to the lowest medium. When the water level reaches -1.2 m, the secondary drainage medium will get active as well. If the groundwater rises above -0.4 m, water will flow towards the drains also. Figures like this can be obtained by field observations and monitoring, or they can be calculated by means of simple or complex equations.

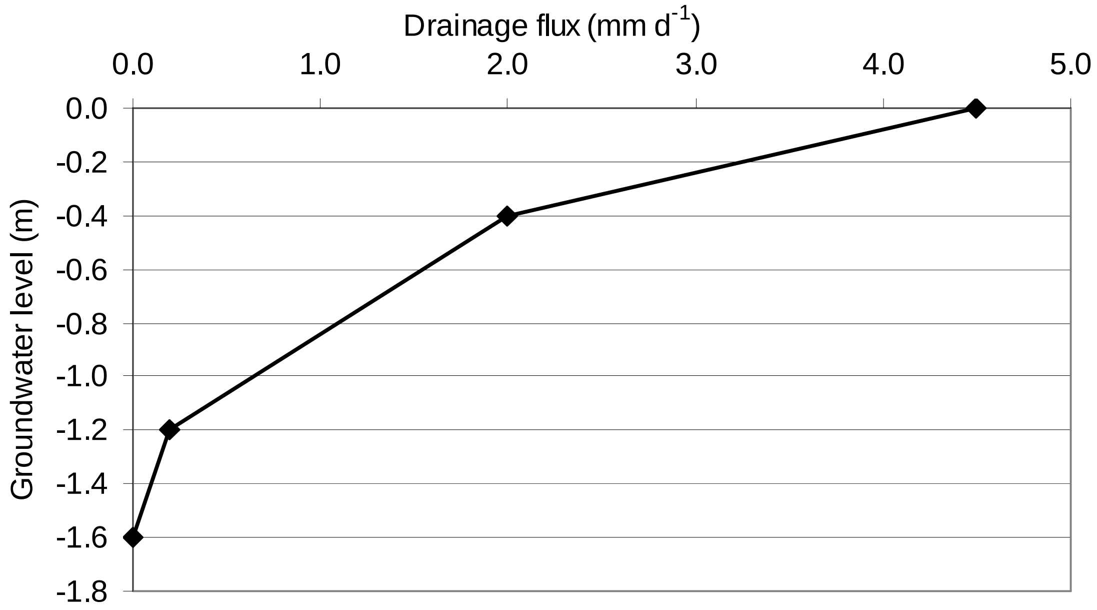


Figure 4.2 An example of a drainage characteristics curve: water flow to the surface water system as a function of the groundwater level.

4.3.3.7 Bottom boundary

Three types of bottom boundary conditions are incorporated in SoWaMCalc. The first type of boundary condition is one where the flux density (q_b, [LT^{-1}]) through the bottom of the profile is computed from the groundwater level (z_g, [L]). The direction of the water flow through the bottom boundary may be upwards (seepage) or downwards (percolation). The relationship between groundwater level and flux density can be defined as a number of (z_g,q_b)-points. An example is presented in Figure 4.3 where the flux is zero when the groundwater level is one meter below soil surface. If the groundwater level is higher (less negative), then water will flow downwards (percolation), otherwise water will flow upward from the deep aquifer (seepage). This kind of relationship is often derived on the basis of field measurements and used in for instance regional studies, see e.g. (Massop et al., 2000).

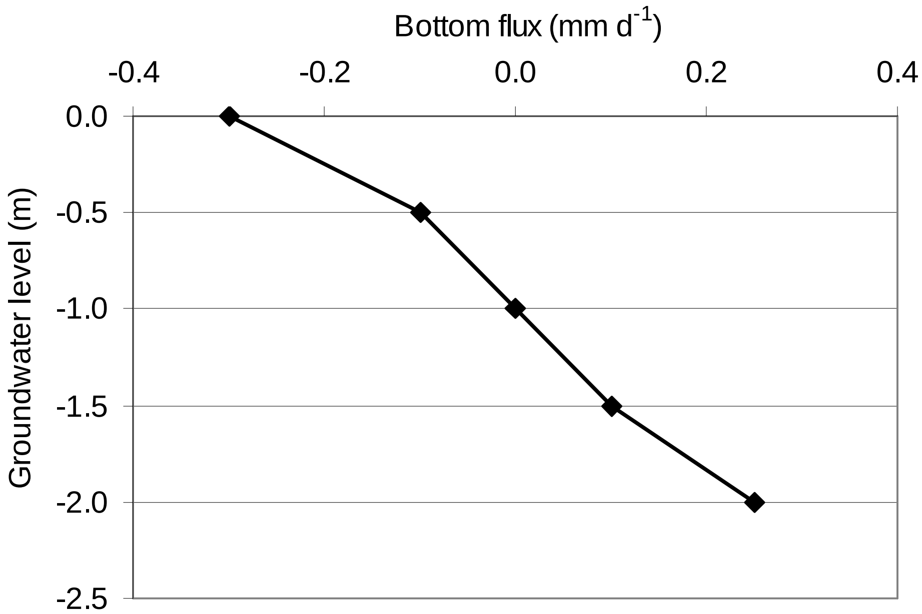


Figure 4.3 An example of a relationship between the flux through the bottom of the profile and the prevailing groundwater level.

The second possible boundary condition in SoWaMCalc occurs when the thickness of the soil profile being considered is small compared to the depth of the groundwater level. If the latter is (virtually) constant at say five meters below the soil surface, and we are only interested in the top two meter, we can assume equilibrium at the bottom of that particular profile. This implies that the gradient of the pressure head equals 1 and that the flux density is equivalent to the prevailing hydraulic conductivity.

The third type of bottom boundary implemented in SoWaMCalc occurs when a relatively fine-textured soil is located on top of very coarse textured layer such as sand or gravel. In such a profile, downward water flow will be hampered until the pressure head at the interface reaches a certain value h_a (cm). In literature the following equation was found (Baker and Hillel, 1990):

$$h_a = -4.37 d^{-1} - 0.074 \qquad (4.13)$$

where d is the median particle diameter (mm). Since SoWaM was initially designed to model water flow in golf greens, the median gravel diameter recommended by the US

Golf Association (USGA Green Section Staff, 2004) was used to calculate h_a. According to these USGA recommendations, 60% of the particles should be between 0.25 and 1 mm, yielding h_a values between -17.5 and -4.44 cm. If this value is reached, free outflow will take place. To avoid unrealistically high amounts of water to flow through the bottom of the profile, the time interval will automatically be assigned to its minimum value when water starts to flow through the bottom of the profile.

4.3.3.8 Irrigation

One of the most important features of SoWaMCalc is its ability to check whether or not irrigation is required for a certain type of crop. To do so, four possible irrigation criteria have been introduced. Irrigation can be applied when

- The ratio of the actual plant evaporation and the potential plant evaporation drops below a specified value,
- The pressure head in a specified node drops below a critical value,
- The moisture content in a specified element drops below a critical value,
- The available volume of water in the root zone is less than a specified value.

It is possible to irrigate more than once a day. The exact time at which irrigation is applied during the day, the duration of the irrigation and the amount of water applied during an irrigation event are user-defined.

4.3.4 SoWaMVis module

As mentioned before, the output of SoWaMCalc is stored in tables in the MySQL-database SoWaMData, thus being directly available to the user. With SoWaMVis, one can visualize these data. Currently three types of output can be generated: i) the flux densities through the top of two user-specified elements can be compared graphically, ii) a term of the water balance can be shown as a graph in time (daily or cumulative values) (Figure 4.4), iii) the pressure heads and moisture contents can be plotted against depth (Figure 4.5), or iv) the moisture volume in the rootzone can be visualized in time together with the distribution of volumes (Figure 4.6).

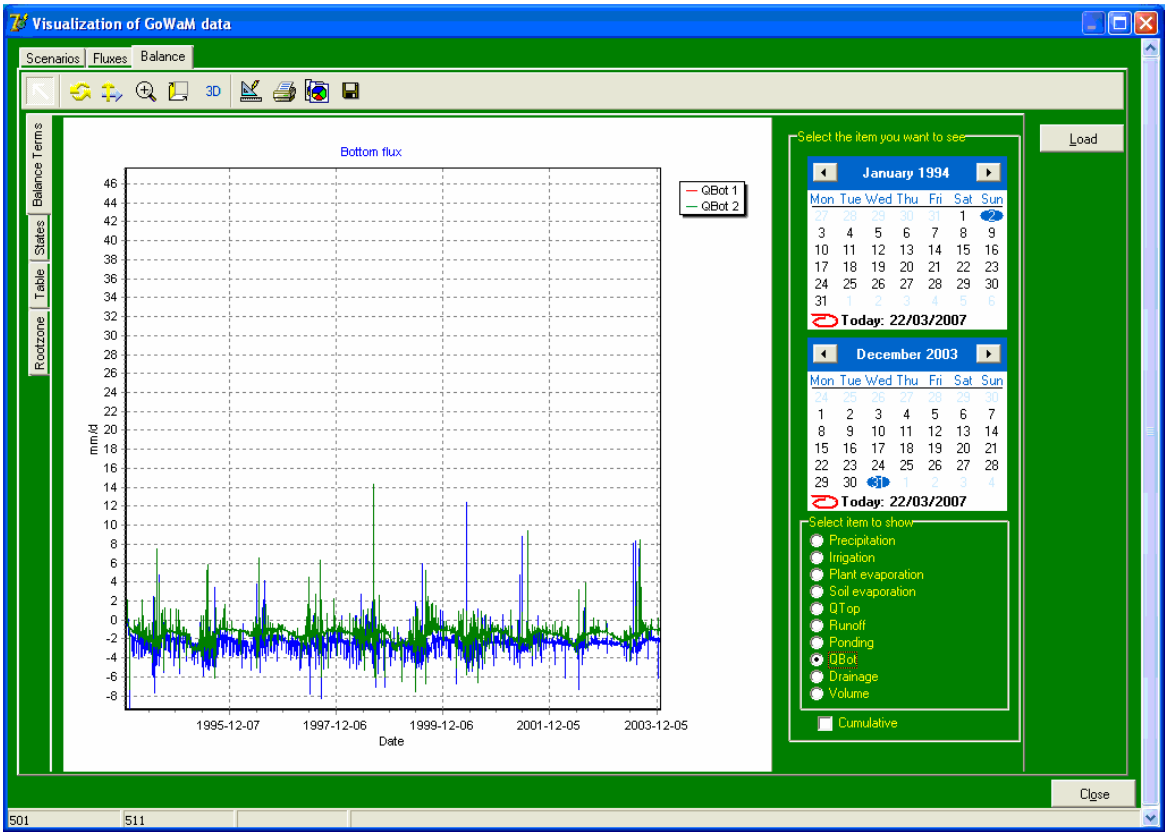


Figure 4.4 An example of the output of SoWaMVis: the water balance terms in time. The start and end date can be selected. One element of the water balance can be visualized at a time for two scenario's. Cumulative values can be shown by clicking the check box 'Cumulative'.

Whatever output option is selected, it is possible to compare the results of two different runs of SoWaMCalc at the same time.

4.3.5 SoWaMSoil module

SoWaMSoil was developed to visualize the soil physical characteristics of the soil layers in the database. When the user selects the name of one of the soil layers in the database, the corresponding soil moisture retention and hydraulic conductivity functions are shown. It works for both the Mualem - Van Genuchten and the spline approximation (Figure 4.7). The resulting curves are presented both graphically and in a table. This table, as others, can be saved as a comma-separated text file for further external processing.

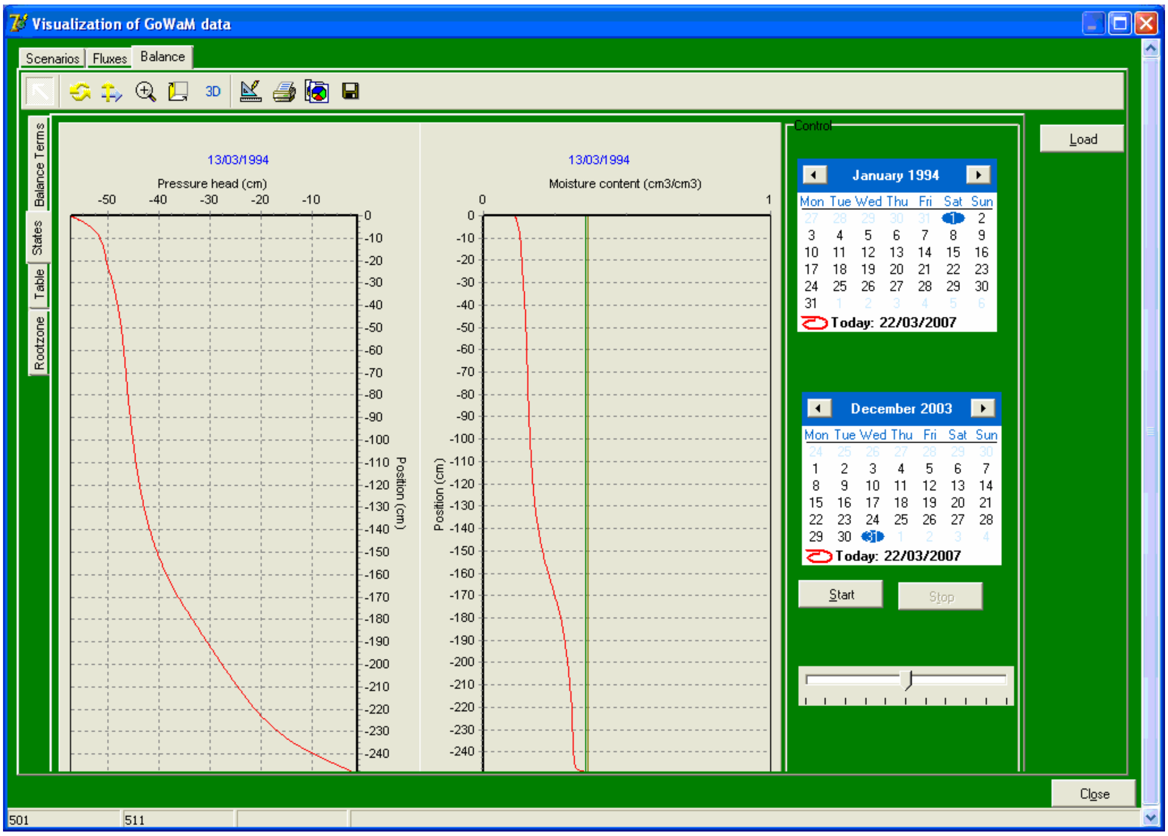


Figure 4.5 Pressure head and moisture content versus depth at a certain date as presented by SoWaMVis. Pressing the 'Start'-button causes the program to show the profiles from the starting day until the end day, thus creating a kind of time animation. The speed of animation can be controlled with the slide-rule at the bottom.

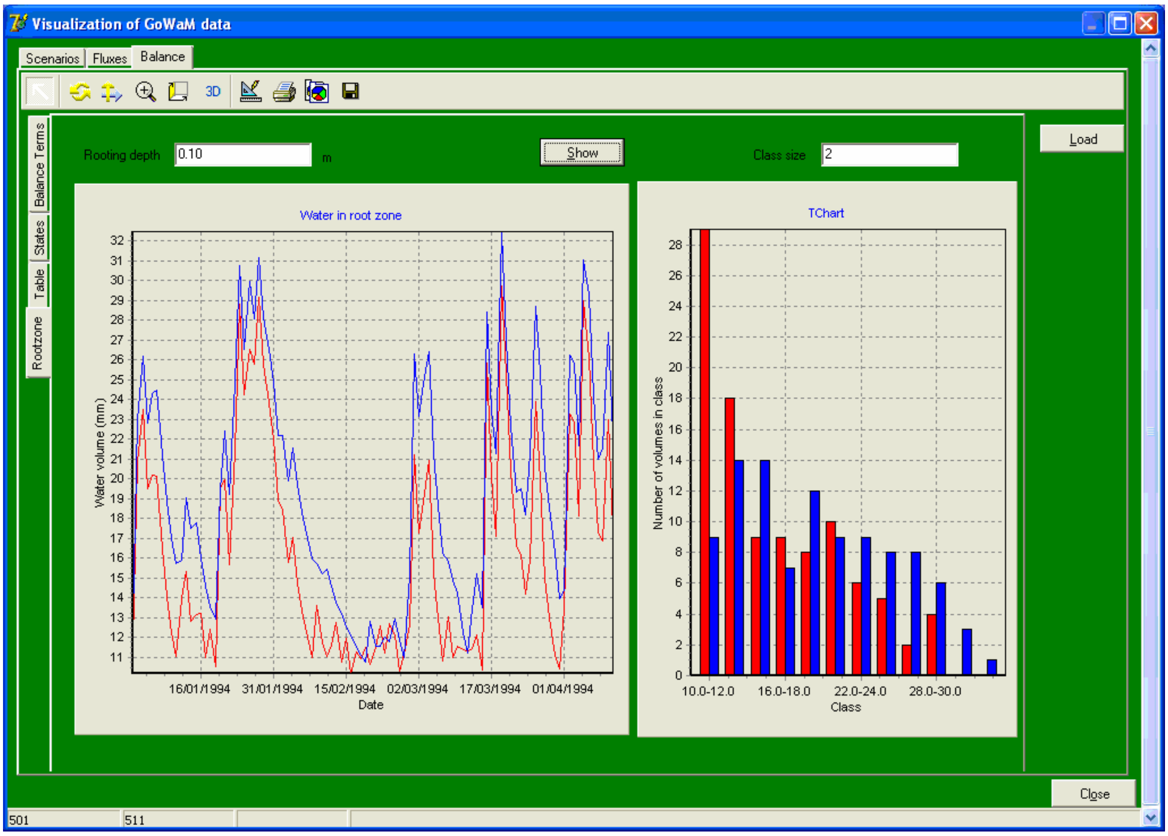


Figure 4.6 The water volume in the root zone of two runs with SoWaMCalc and the frequency distribution of computed classes of water volume as shown by SoWaMVis. The thickness of the root zone to be considered in calculating these figures can be changed at the top left. The class-size can be changed at the top right.

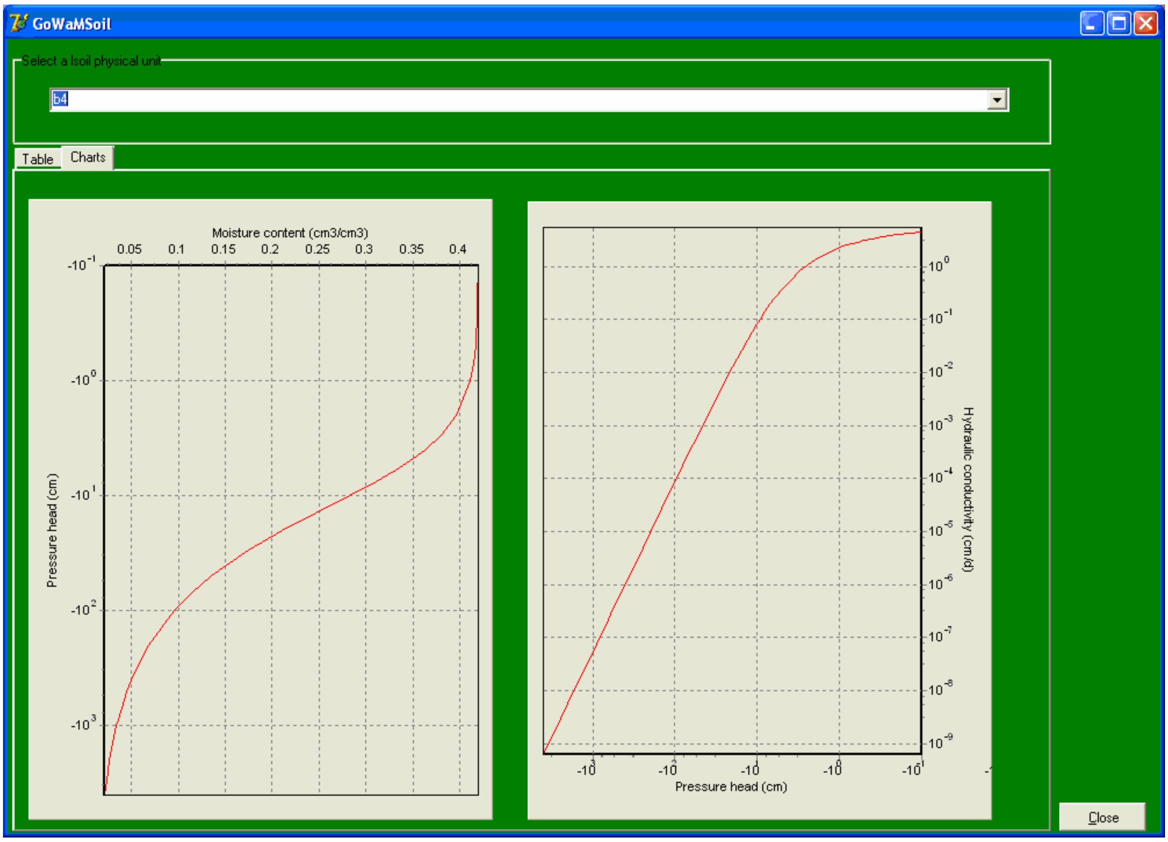


Figure 4.7 The program SoWaMSoil shows the soil physical relationships h(θ) (left) and K(h) (right) of a soil layer in the database.

4.3.6 SoWaMFit module

Based upon the program Splop (Wesseling et al., 2008b), SoWaMFit fits a number of splines through a set of measured data points of the soil moisture retention curve and the hydraulic conductivity function (Figure 4.8). The resulting output can be directly stored into the SoWaMData database.

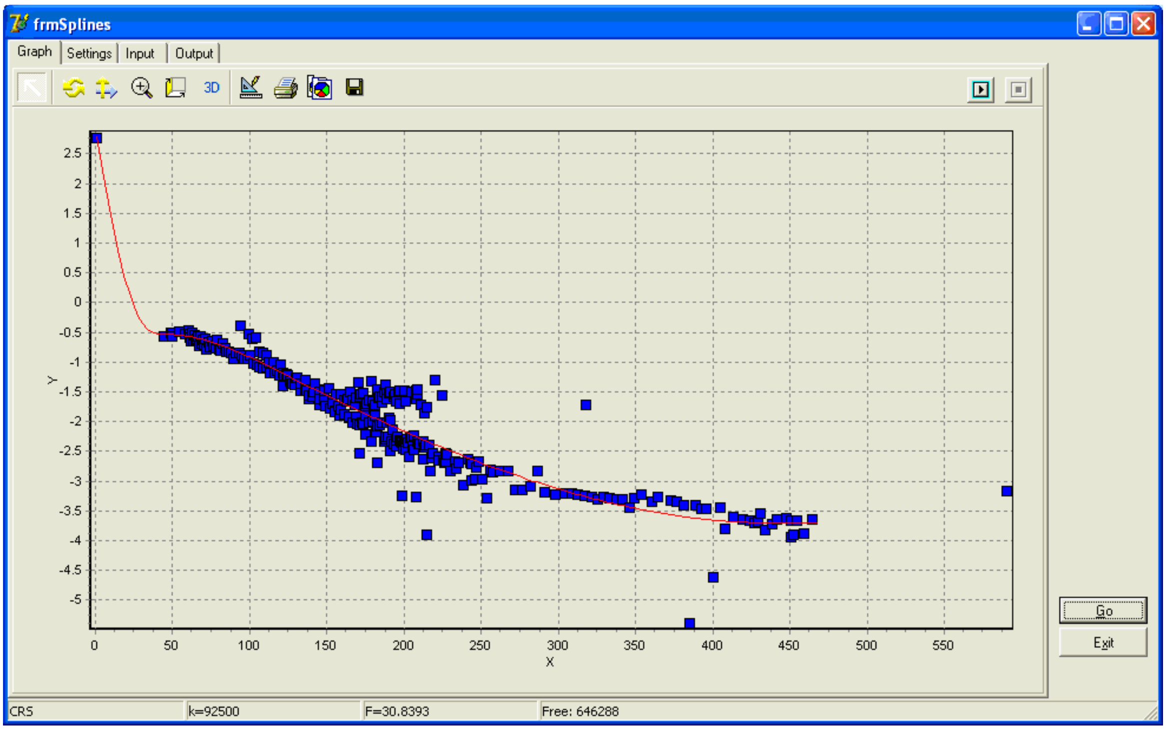


Figure 4.8 An example of the results of SoWaMFit. As this program is generally applicable for fitting of splines, only x and y are put at the axes. In this case, pressure head is plotted on the x-axis, while hydraulic conductivity is plotted on the logarithmic y--axis. The squares indicate measured K(h)-values, the line is fitted by the program.

4.3.7 SoWaMDrain module

The relationship between groundwater level and drainage intensity can be obtained by SoWaMDrain. Its output looks like Figure 4.9.

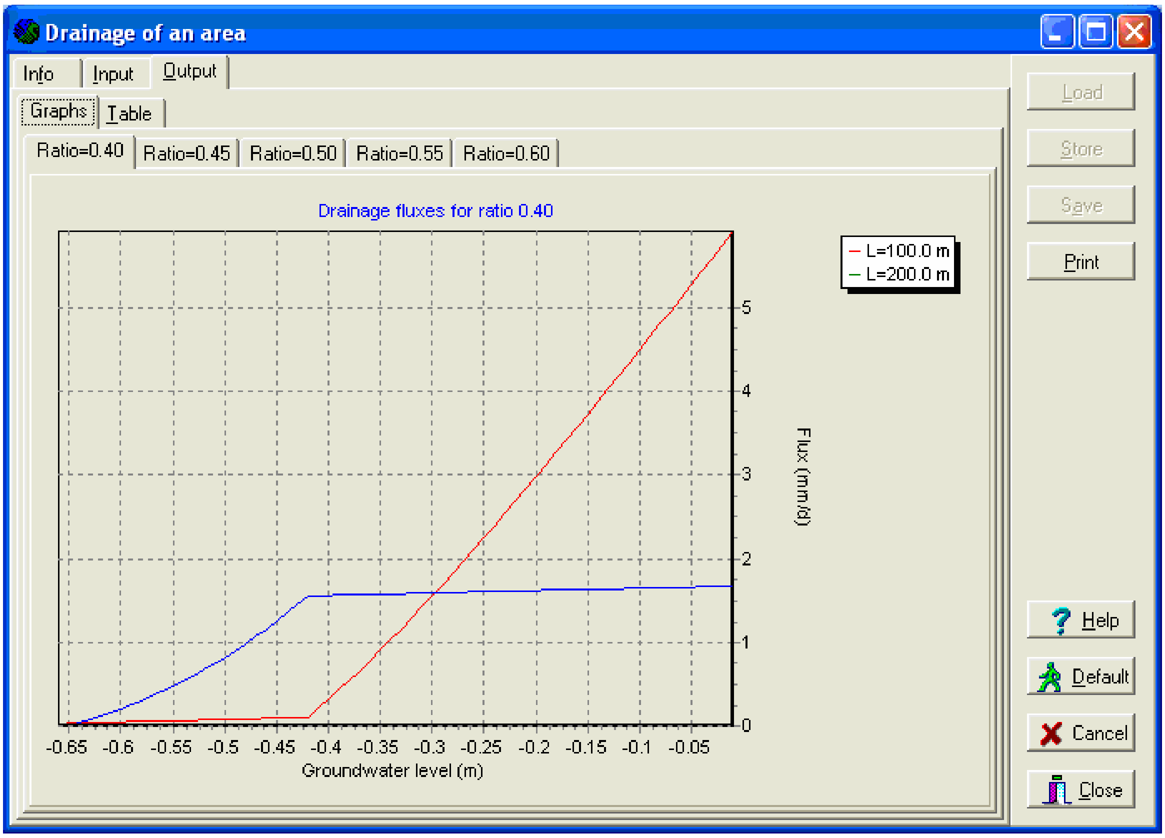


Figure 4.9 An example of the drainage fluxes with two different drainage distances (L=100 m and L=200 m) as calculated with SoWaMDrain.

4.4 Comparison of SoWaM to other models

In this section we compare the SoWaM model with several other well-known 1-dimensional soil water flow models, namely Ecoul (Perrier et al., 2002), SWAP (Van Dam et al., 1997b) and Hydrus-1d (Simunek et al., 1998). Similarities and differences between SoWaM and these other models are summarized in Table 4.1.

Table 4.1 Comparison of four different models for one-dimensional moisture flow. Presence (+) and absence (-) of several model features are summarized for each of the models.

Feature	Hydrus-1D	Swap	Ecoul	SoWaM
Basic model approach				
Use of Richards equation	+	+	+	+
Calculation time steps	Fraction of day	Fraction of day	Fraction of day	Nmber of seconds
Maximum number of nodes	Unlimited	500	unlimited	unlimited
Varying boundary conditions	+	+	+	+
Processes				
Surface ponding	+	+	+	+
Root water uptake	+	+	-	+
Crop growth	-	+	-	+
Automated irrigation	-	-	-	+
Macropore flow	+	+	-	-
Breakthrough to coarse layer	-	-	-	+
Drainage	+	+	-	+
Soil layers				
Max. soil layers	unlimited	40	unlimited	unlimited
Van Genuchten-Mualem equations for hydraulic properties	+	+	+	+
Spline interpolation of soil hydraulic properties	-	-	-	+
Input/output				
Database-IO	-	-	-	+
Batch	-	+	-	+
GUI	+	-	+	+
Tabulated hydraulic properties	-	-	-	+
Tabulated drainage curve	-	-	-	+
Specify time of day for irrigation	-	-	-	+
Irrigate more than once a day	-	-	-	+
Visualization of results from several runs	-	-	-	+

It can be seen that SoWaM has only a restricted amount of model options compared to the Swap and Hydrus-1d models, just like Ecoul. However, the main advantages of SoWaM compared to the three other models are i) time intervals of seconds versus days, ii) automatic irrigation control, iii) breakthrough to coarse layers, iv) spline interpolation of soil hydraulic properties, v) data input from and output to a database, vi) tabulated hydraulic properties and drainage curves, vii) specification of times of day for irrigation, viii) option to irrigate more than once a day and ix) simultaneous visualisation of results from multiple runs.

4.5 Conclusions

To conclude, the SoWaM package has the following benefits:

- It is a simple yet highly flexible model with the following advantages i) very small calculation intervals, ii) automated irrigation control, iii) breakthrough to coarse layers, iv) spline interpolation of soil hydraulic properties, v) database IO, vi) tabulated hydraulic properties and drainage curves, vii) specification of time of day for irrigation, viii) option to irrigate more than once a day and ix) visualisation of results from different runs.
- Due to its object-oriented structure it is quite easy to add new model options.
- No complex boundary conditions have to be introduced.
- It can be used to compute soil moisture flow in a (both temporally and spatially) detailed manner.
- Data are stored in and read from an open-source MySQL database.
- Data are readily available for post processing.
- SoWaM is suitable for batch processing.

5 The effect of soil texture and organic amendment on the hydrological behavior of coarse-textured soils

To gain more insight in the hydrological behavior of coarse-textured soils, the physical properties of artificially created soil mixtures with different texture were determined. The mixtures were prepared according to the USGA specifications for constructing putting greens. Additionally, the effect of 10 vol. % organic matter addition was studied. The soil moisture retention and hydraulic conductivity relationships of the different mixtures were measured and their hydrological behavior was studied using the numerical model SoWaM. Both texture and organic matter addition considerably affected hydraulic properties. Hydraulic conductivity significantly increased with increasing coarseness while moisture retention decreased. On the other hand, organic matter addition reduced saturated hydraulic conductivity with a factor 10 to 100 and it increased moisture retention capacity distinctly. The amounts of readily available water were increased with 144% (slightly coarse texture) to 434% (very coarse texture) for the samples with 10 vol% organic matter. Model simulations show that the required amount of irrigation to keep sport turf healthy strongly differs between the mixtures, despite that all samples fall in the range of official USGA-specifications.

Adapted from

Wesseling, J.G., C.R. Stoof, C.J. Ritsema, K. Oostindie and L.W. Dekker. 2009. The effect of soil texture and organic amendment on the hydrological behavior of coarse-textured soils. Soil Use and Management. In Press.

5.1 Introduction

In previous chapters an universal way to describe the physical properties of a soil by means of a fitting procedure using cubical splines (Wesseling et al., 2008b) was presented, the risks of clustering soil samples into soil physical classes (Wesseling et al., 2009b) were emphasized and a new and flexible computer program to simulate one-dimensional moisture flow (Wesseling et al., 2009c), was introduced. While developing and testing these methods and tools, the soil physical properties of a wide range of soils were required. Nowadays both raw data of soil physical relationships, averaged characteristics and more generic pedotransfer functions can be found in different databases, like the Staring Series (Wösten, 1987; Wösten et al., 2001b), the UNSODA database (Nemes et al., 2001), the Hypres database (Wösten et al., 1998; see http://www.macaulay.ac.uk/hypres/) and the Priapus database (Stolte et al., 2007). Searching these databases and the scientific literature yielded surprisingly little data on the soil physical properties of coarse-textured soils. A quick literature search showed that these kinds of soils have been investigated in combination with transport of NO_3 (Dodd et al., 2000), microbiology (Kieft et al., 1995), gas diffusion (Jones et al., 2003), the amendment of fly ash (Adriano and Weber, 2001), waste water (Harrison et al., 2000) and earthworms (Zhang and Schrader, 1993), but hardly any measurements were performed on the soil physical properties of these types of materials. This is rather surprising, the more when one realizes that 3.5% of the Dutch topsoils have a median particle size of 210 µm or higher (the Dutch definition of coarse sand). Coarse soil materials usually have limited possibilities for agricultural production due to their generally poor fertility and low water holding capacity, often causing a high irrigation demand.

Despite this fact, coarse textured soils are frequently used worldwide because of their good drainage and low risk of compaction, for instance to construct greens on golf courses. Golf greens are constructed most often using sand brought in from elsewhere with properties in accordance with the US Golf Association specifications regarding texture composition (USGA Green Section Staff, 2004). Even though different sand mixtures yield different water holding capacities on golf courses (Chong et al., 2002), these specifications mainly aim at achieving optimal drainage characteristics while monitoring optimal grass growth conditions (Hummel, 1993). Depending on the geographical location of a golf course and the climatic conditions, the amount of water required for irrigation of golf courses can vary from 50,000 to 100,000 m^3y^{-1}.Though papers have been published on designing strategies to save irrigation water on golf courses (Carrow, 2006; Carrow et al., 2002a; Carrow et al., 2002b), no research has been performed up to now to evaluate different USGA mixtures regarding their hydrological performance including related irrigation requirements. Though the influence of soil materials and slope of the green on drainage have been investigated experimentally for putting greens built with a Californian (coarse material, densely drained, on top of local material) and a USGA construction method (coarse material, densely drained, on top of at least 0.1 m of gravel) (Prettyman and McCoy, 2002), better insights are urgently needed to minimize irrigation requirements and reduce leaching risks of nutrients and pesticides.

This study (Wesseling et al., 2009a) combines an extensive laboratory study with a detailed numerical evaluation of flow and transport behavior of a series of coarse-textured soil materials that comply with the USGA-specifications. This Chapter first describes the soil mixtures used and the determination and interpretation of the related hydraulic conductivity and water retention characteristics. Further, simulation results using the numerical model SoWaM (Wesseling et al., 2009c) are presented and interpreted in relation to the different terms of the water balance. Two types of soil profiles are considered in this study: i) a homogeneous profile of 2.5 m deep, and ii) a 30 cm coarse top layer upon gravel, as recommended for putting green construction by the USGA-specifications.

5.2 *Materials and methods*

5.2.1 The sand mixtures

In this study, five sand mixtures were created ranging from slightly to very coarse textured using sand sieved in different particle size classes which was obtained from the company Filcom (Barendrecht, The Netherlands). The sand mixtures prepared complied with the USGA specifications for golf green construction (USGA Green Section Staff, 2004) (Table 5.1).

Table 5.1 USGA recommendations for soil texture (USGA Green Section Staff, 2004)

Material	Particle diameter (mm)	Recommended fraction (%)	
Fine gravel	2.0 – 3.4	< 3	} < 10
Very coarse sand	1.0 – 2.0	-	
Coarse sand	0.5 – 1.0		} > 60
Medium sand	0.25 – 0.50		
Fine sand	0.15 – 0.25		< 20
Very fine sand	0.05 – 0.15	< 5	} < 10
Silt	0.002 – 0.05	< 5	
Clay	<0.002	< 3	

For preparing the sand mixtures, five particle size distributions were selected covering the entire textural range from the finest (Sample A) to the coarsest recommended texture (Sample E, Table 5.2). Two types of homogeneous sand mixtures were constructed: 1) non-amended sand mixtures containing only mineral components (hereafter referred to as ‘pure’), and 2) peat-amended sands containing both mineral and organic components (‘amended’). The peat amended sands contained 10% by volume fine-grained peat (98% organic matter as determined by loss on ignition), corresponding with 7% organic matter on weight basis. The mixtures were prepared by mixing homogeneous materials of different particle size. The amount of each fraction was calculated from the desired particle size distribution (Table 5.2) and a porosity of 35%. Particle density was assumed to be 2.65 g cm^{-3} (sand) and 1.47 g cm^{-3} (peat) (Werkgroep Herziening Cultuurtechnisch Vademecum, 1988).

Table 5.2 Particle size distribution of constructed sand mixtures (%)

Texture	Particle diameter (mm)						
	2.0–3.4	1.0–2.0	0.5–1.0	0.25–0.50	0.15–0.25	0.05–0.15	< 0.05
A	0	0	0	70	20	5	5
B	0	0	20	55	15	5	5
C	1.5	3.5	40	40	10	2.5	2.5
D	2.25	5.25	65	20	5	1.25	1.25
E	3	7	90	0	0	0	0

PVC cylinders (103 mm diameter, 80 mm height) lined with cheesecloth were manually filled with the sand mixtures, attempting to ensure uniform density. The samples were slowly saturated from the bottom up for at least 72 hours. All measurements were performed in a climate-controlled laboratory with air temperature between 16 and 17°C and relative humidity between 65 and 70%.

5.2.2 Soil physical relationships

Saturated hydraulic conductivity (K_{sat}) was measured on the saturated sand mixtures (3 replicates per treatment) using the constant head method as described by Stolte (1997). Consequently, water retention and hydraulic conductivity characteristics were determined on the same samples using Wind’s evaporation method (Wind, 1966). According to this method, a saturated soil sample is placed on a scale for monitoring weight loss due to evaporation, while ceramic tensiometers monitor changes in soil water pressure at different depths. The tensiometers used in this study were relatively large (8 mm in diameter, 8 cm in length) to ensure sufficient contact between the tensiometer and the coarse-textured soil material mixtures. Data in the pressure head range of -800 cm to 0 cm was gathered for all samples except for mineral sample E where air entered the tensiometers at a pressure head h of -300 cm for all three replicates. Obtained $h(\theta)$ and $K(h)$ data from the Wind evaporation method (Stolte and Veerman, 1990) were used to determine the water retention and unsaturated hydraulic conductivity characteristics. These data were further processed and relationships were obtained by using the recently developed spline-fitting method of Wesseling et al. (2008b). The minimal MDPL (Mean Distance from Point to Line) was applied for this purpose, offering more flexibility in fitting than the often used Mualem - Van Genuchten method, as well as that it takes K_{sat} better into account.

5.2.3 Model simulations

5.2.3.1 Profiles

Two types of soil profiles are considered in the modeling part of this study (Figure 5.1). The first type is a homogeneous soil profile of 2.5 m thickness with a constant groundwater level at the bottom of the soil profile. The second profile consists of a 30 cm surface layer on top of a gravel layer. For this profile it was defined that water could flow from the sand to the gravel only at pressure heads at the interface exceeding -10 cm (Baker and Hillel, 1990). If this critical pressure head is reached, free outflow takes place until the pressure head drops again below this critical value.

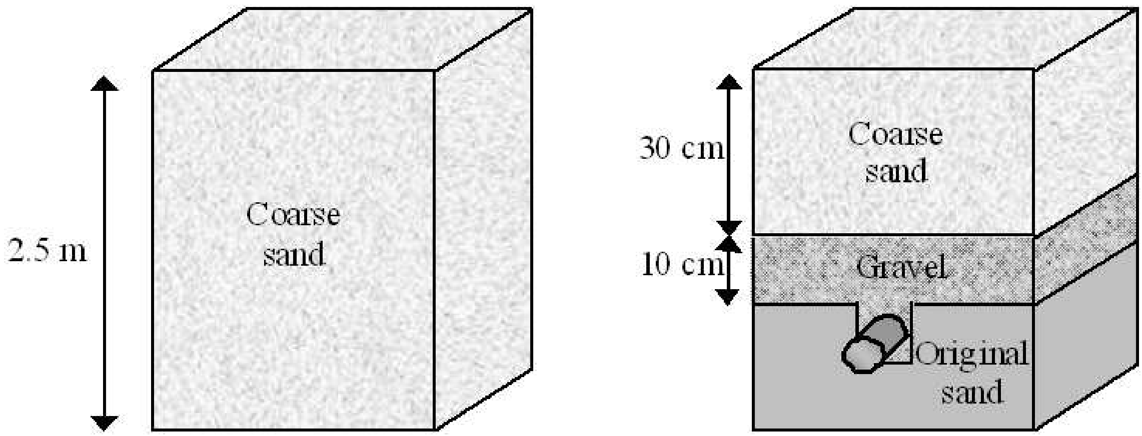


Figure 5.1 Two types of profiles used for evaluating the hydrological behavior of the coarse textured mixtures.

5.2.3.2 Meteorological data

For an 11-year period, 1994-2004, covering wet, average and dry years (Wesseling et al., 2007), model simulations have been performed. Precipitation and potential evaporation data (on a 6-hour basis) have been obtained from the meteorological station of Wageningen University (www.met.wau.nl). Figure 5.2 shows the precipitation and potential evaporation amounts against time. For the sake of simplicity only the average monthly values have been used for constructing Figure 5.2.

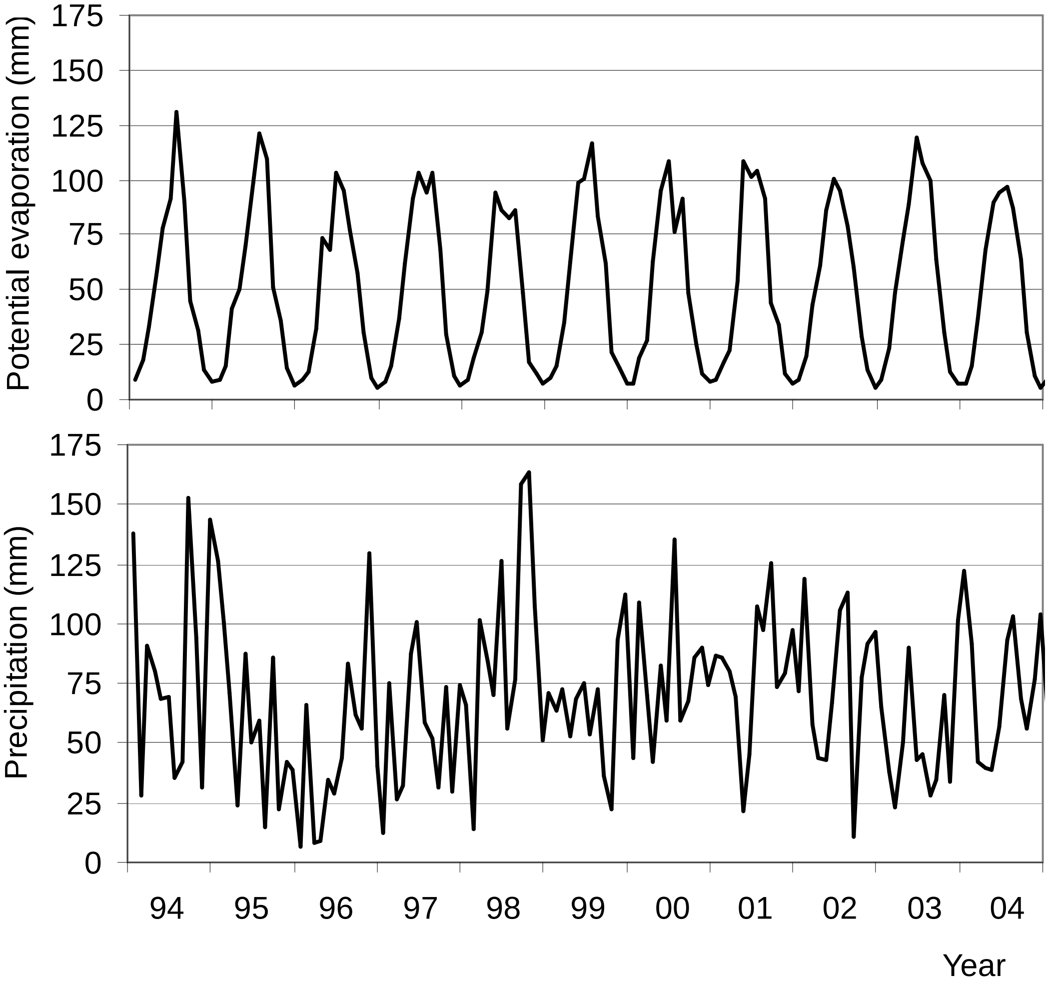


Figure 5.2 The monthly values of potential evaporation and precipitation from the meteorological station of Wageningen University and Research Centre for the years 1994-2004 (after Wesseling et al., 2007).

5.2.3.3 Crops

The considered crop in the modeling simulations is grass. The rooting depth was assumed to be 0.05 m with roots uniformly distributed over this rooting zone. The Leaf Area Index was kept constant and set to 2 m^2m^{-2}, because grass is mowed frequently on golf courses, sometimes daily. Plant evaporation is dependent on the prevailing pressure head in the root zone (Feddes et al., 1978; Van Dam et al., 1997b; Wesseling et al., 2009c). In this study, it is assumed that the root water uptake is zero when the pressure head is higher than -10 cm (wetness stress), or lower than -8000 cm (drought stress). Root water uptake is optimal for pressure heads between -25 cm and -200 cm.

5.2.3.4 Irrigation requirement

The model SoWaM offers a lot of possible irrigation criteria (Wesseling et al., 2009c), such as the ratio between the actual and the potential plant evaporation, a threshold value for the moisture content at the centre of the root zone, a threshold value for the pressure head at a specified depth, and the amount of available soil water in the rootzone. In this study the transpiration ratio was used to trigger irrigation.

5.2.3.5 Available output

Simulation runs with SoWaM (Wesseling et al., 2009c) provide a lot of data, stored in a database automatically, like all terms of the water balance, required irrigation amounts, and data showing the computed pressure head or moisture content versus depth and time. Output data can be stored for each timestep, but also for instance at the end of a simulated day only.

5.3 Results and discussion

5.3.1 Characteristics of the samples

5.3.1.1 Bulk density and porosity

Dry bulk density and total porosity were determined for the constructed root zone mixtures, see Table 5.3. Dry bulk density ranged from 1.64 to 1.75 g cm^{-3} for the pure mineral samples and from 1.59 to 1.61 g cm^{-3} for the amended samples. Amended samples always had lower dry bulk densities.

Table 5.3 Bulk density and porosity of the 5 mixtures

Sample	Bulk density g cm^{-3}		Porosity %	
	Pure	Amended	Pure	Amended
A	1.69	1.59	35.4	37.3
B	1.75	1.61	31.9	36.2
C	1.73	1.60	32.9	37.1
D	1.72	1.60	33.5	36.9
E	1.64	1.61	38.4	36.4

The porosities of the pure samples ranged from 31.9% to 38.4%, for the amended from 36.2 to 37.3%. Porosities of amended samples were always higher than for the related mineral samples, except for the coarsest E sample.

5.3.1.2 Saturated hydraulic conductivity

The measured saturated hydraulic conductivity was high for all pure samples, up to 160 m d^{-1} for the coarsest sample E (Figure 5.3). All samples fulfill the requirements of the USGA for putting green construction, where it is advised to use soils with K_{sat}–value higher than 3.6 m d^{-1} (USGA Green Section Staff, 2004). Measured K_{sat}–values of the amended samples was considerably lower compared with the pure samples, K_{sat} roughly decreased by a factor 10 to 100 to values of 0.8 to 1.6 m d^{-1} (Figure 5.3). K_{sat}–values are all in the same range for the amended mixtures with values just below the recommended value of 3.6 m d^{-1} of the USGA.

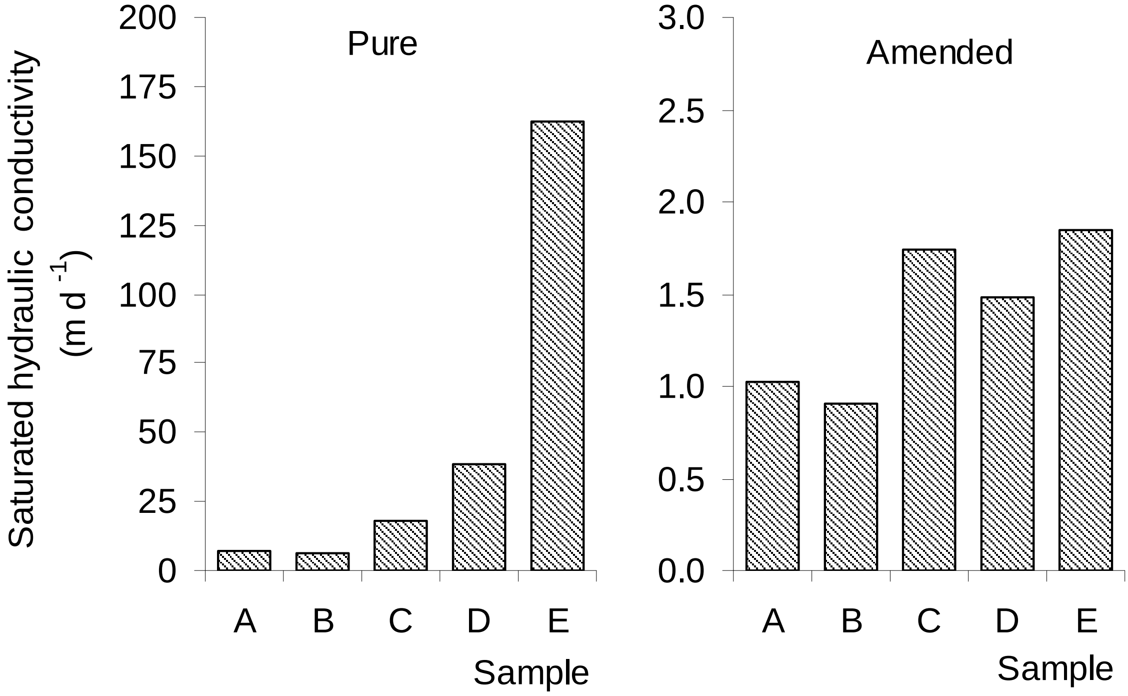


Figure 5.3 Measured saturated hydraulic conductivity of pure and amended samples. Please note that the y-axes have different scales.

5.3.1.3 Unsaturated hydraulic conductivity

The unsaturated hydraulic conductivity curves were fitted using the K(h) data obtained by the Wind measurements (Stolte and Veerman, 1990) and the average of the three K_{sat} values measured with the constant head method (for h = 0 cm) (Stolte, 1997) . The fitting program Splop (Wesseling et al., 2008b) allows to fix the value of K_{sat}. In this study we fixed it at the values presented above. As an example, Figure 5.4 presents the results of the fitting program for the relationship between the pressure-head and hydraulic conductivity of the pure C-sample.

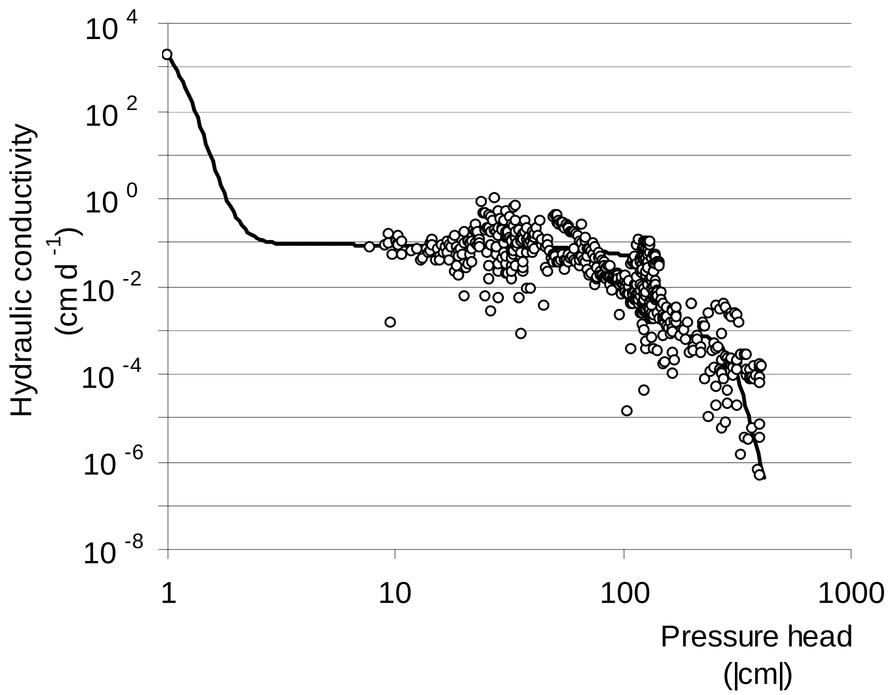


Figure 5.4 Results of the fitting-program Splop.exe, yielding the fitted line through the measured points of the pressure head [cm] (x) versus hydraulic conductivity relationship [cm d^{-1}] (y) of the pure C-sample.

The measured data sets contain only few K(h)-points for pressure head values in the range between 0 and -40 cm. This was caused by the fast outflow of water when inserting the tensiometers in the fully saturated soil sample. In this pressure head range, the shapes of the fitted hydraulic conductivity curves are therefore entirely dependent on mathematical interpolation.

Figure 5.5 shows the hydraulic conductivity functions of all mixtures against pressure head. The curves of the amended samples look more or less the same. For the pure, mineral samples, mixtures A and B have the same shape roughly, while differences occur for increasingly coarser mixtures.

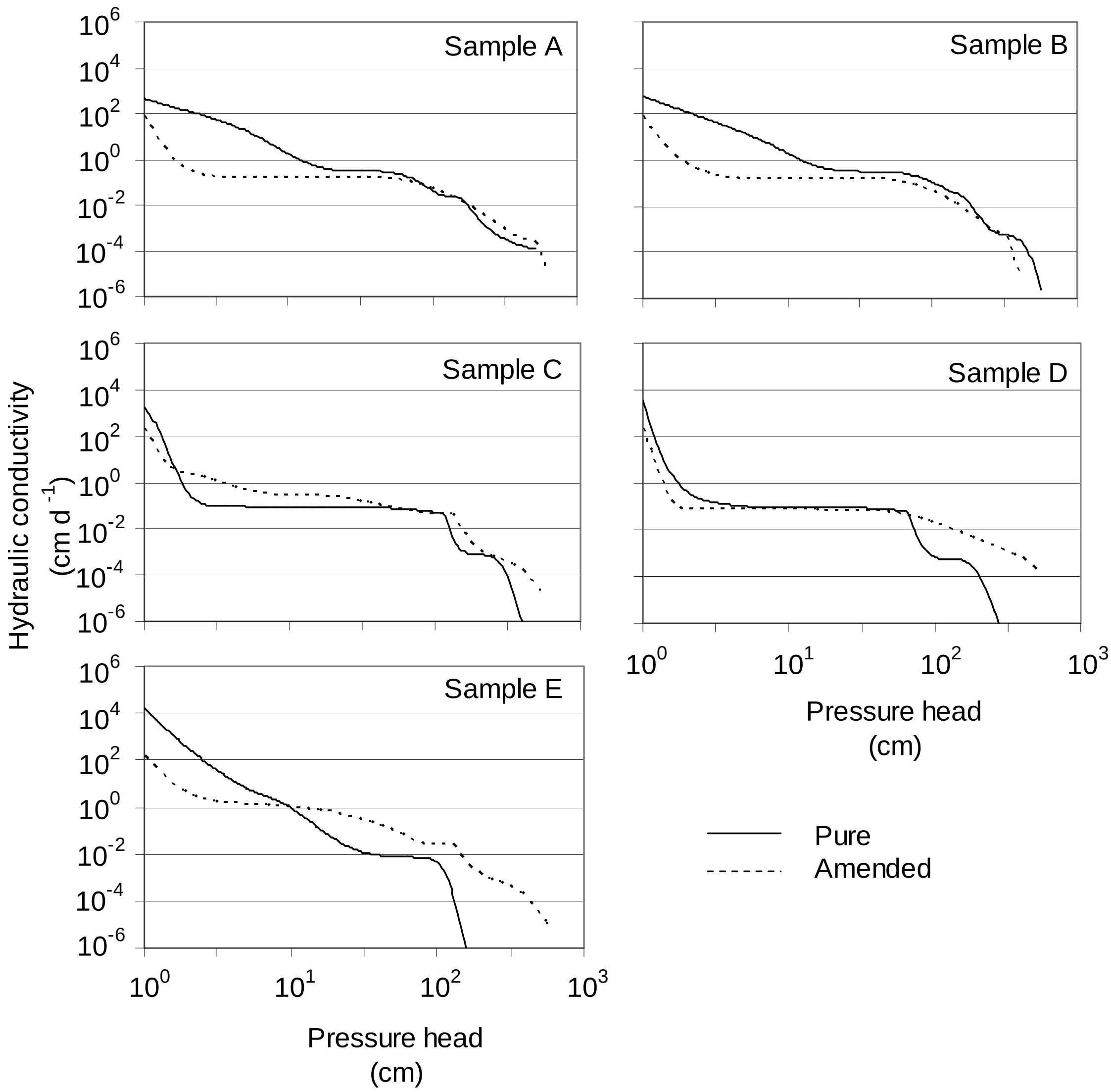


Figure 5.5 Unsaturated hydraulic conductivity curves for the pure and amended samples A (fine-textured) to E (coarse-textured).

5.3.1.4 Water retention

The water retention curves were fitted using the h(θ) data obtained by the Wind measurements and the measured total porosity (equaling θ_{sat}, for h = 0 cm). Since current tensiometers fail to measure below h < -850 cm, there is also little data of the dry part of the curve (θ < 0.02 to 0.04 for the pure mixtures; θ < 0.07 to 0.09 for the amended mixtures). Also in the wettest part (θ > 0.32 to 0.34), few data are available due to rapid outflow of water before installing the tensiometers in the samples.

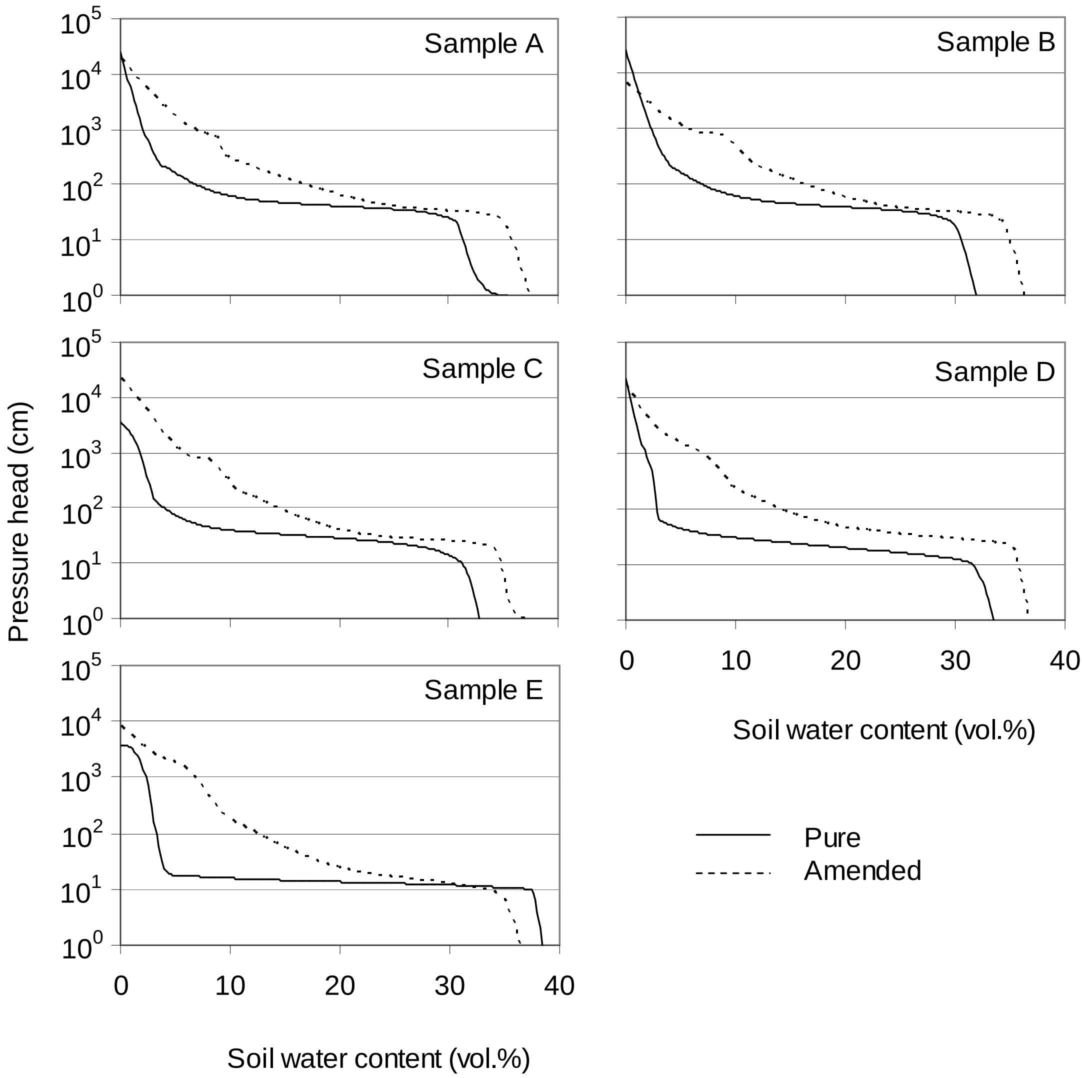


Figure 5.6 Measured water retention curves for samples A (fine-textured) to E (coarse-textured).

The water retention curves of the pure samples (Figure 5.6) show that for soil moisture contents between 0.04 and 0.3, the amount of moisture retained at a certain pressure head increases with decreasing particle size. In addition, the shape of the curves shows that mixtures of fine-textured materials retain more water and drain their water more gradually than mixtures with coarse-textured materials. The shapes of the curves of the amended mixtures are almost similar, with little actual differences. It can be seen that addition of 10 vol. % organic matter increases the amount of water retained, almost independently of related pressure head.

5.3.1.5 Readily available water

A commonly used indicator is the RAW (Readily Available Water) value, being the amount of water that is stored between field capacity (h=-100 cm) and wilting point (h=-16,000 cm). These values are presented in Figure 5.7, where it is shown that the addition of organic matter results in a significant increase in the amount of readily available water. Adding 10% organic matter to the soil samples increased the amount of readily available water with 144% (texture B) to 434% (texture D), respectively.

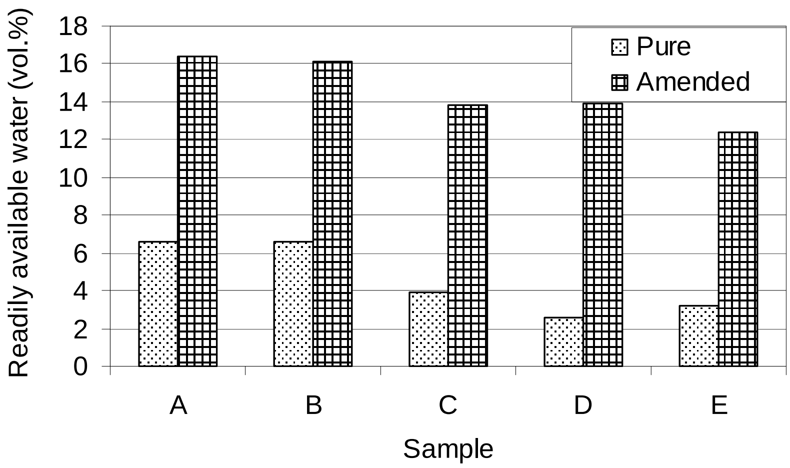


Figure 5.7 The readily available water for the pure and amended soil samples.

5.3.2 Model simulations

5.3.2.1 Uniform soil profiles

Model simulations over an 11-year period (1994-2004) were performed for 10 homogeneous soil profiles consisting of the pure mineral mixtures and the mixtures amended with organic matter. Two simulation runs have been executed, one without and one with the activation of the irrigation criterion. In the latter case, irrigation is applied when plant evaporation ratio (= actual plant evaporation / potential plant evaporation) drops below 0.9. Irrigation is then applied at 7 AM during 30 minutes, totaling an amount of 4 mm. For both simulation runs (with and without irrigation) the terms of the water balance have been determined. In Figure 5.8 the ratio of actual and potential plant evaporation is shown for both simulation runs. The ratio varies from 0.27 (D) to 0.44 (B) for the mineral soils and from 0.36 (E) to 0.46 (D) for the amended soils. Applying irrigation results in ratios varying from 0.44 (E) to 0.76 (C) for the mineral soils and from 0.59 (E) to 0.67 (D) for the soils with amendments.

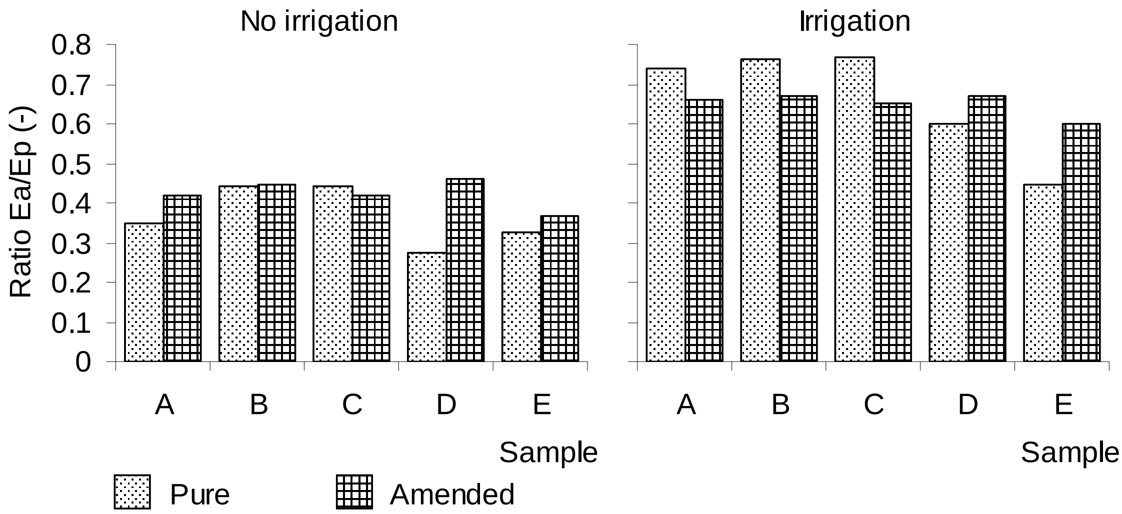


Figure 5.8 The ratio of actual and potential plant evaporation for the mineral and the amended homogeneous soil profiles with and without irrigation.

From these data it can be concluded that the applied amount of irrigation water was apparently insufficient to achieve optimal water uptake by the grass. This might be caused by the fact that at least part of the applied irrigation water leached rapidly through the rooting zone of the respective mixtures immediately after application, maintaining the water stressed situation during the day and leading to low ratios of actual to potential plant evaporation.

Figure 5.9 shows the yearly irrigation totals as computed by the model. Irrigation amounts for mineral soils are higher than the amended soils, except for the E-mixture. The required amount of irrigation for the mineral mixtures varies between

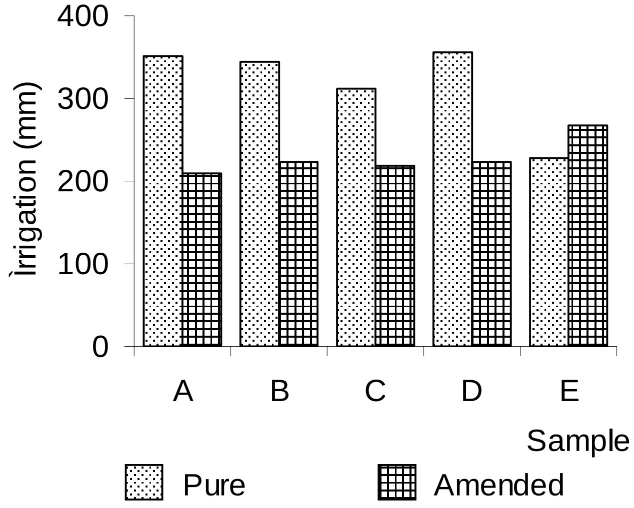


Figure 5.9 The yearly irrigation supply for the 5 soil profiles with and without amendment. Values are averaged over the period 1994-2004.

228 mm for the E-mixture and 355 mm for the D-mixture. In case of the amended soil mixtures, the yearly irrigation varies between 210 mm (A) and 268 (E) mm. This implies an average irrigation reduction of around 35% for profiles A-D, but a slight increase of 17% for profile E.

In Figure 5.10 the computed water losses through the bottom of the soil profiles (2.5 m) are shown. It can be concluded that i) amended mixtures have lower water losses to the subsoil and ii) irrigation of mineral soils lead to higher water losses compared with no irrigation conditions. This is not necessarily the case for the amended mixtures.

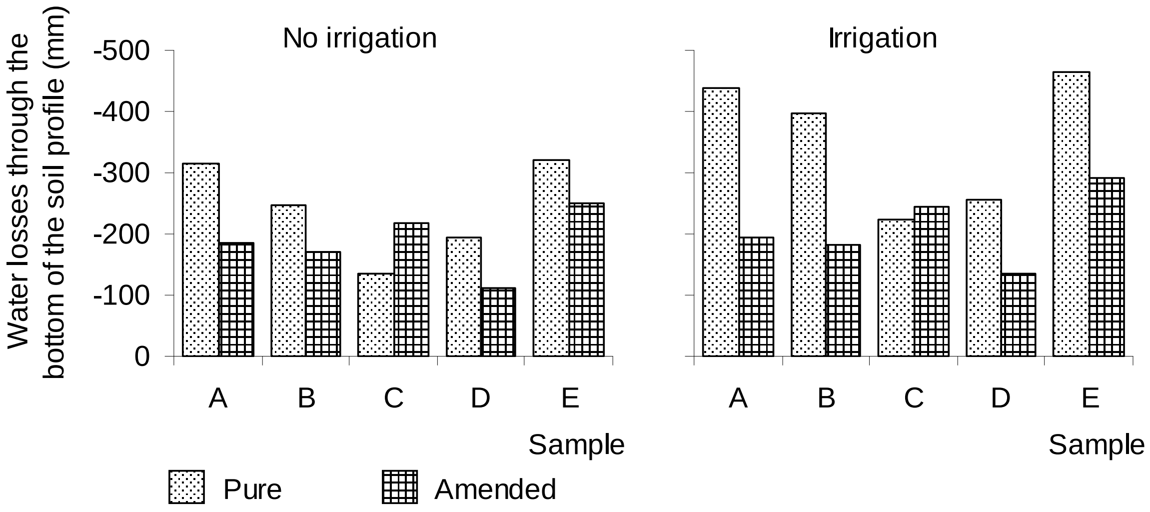


Figure 5.10 The yearly flux through the bottom (2.5 m) of the 5 soil profiles with and without amendment. Values are averaged over the period 1994-2004.

5.3.2.2 Soil profile on a layer of gravel

Calculations were performed for one year (1994, a 6% dry year) again, but now a 30 cm thick soil layer on top of a layer of gravel was assumed. All soil materials discussed in the previous paragraphs were applied again. Though we were mostly interested in the effects of soil texture and amendment on irrigation requirement, we also had the opportunity to mutually compare both profiles.

The same irrigation scheduling was applied in this case. The applied yearly irrigation is presented in Table 5.4.

Table 5.4. Irrigation requirements (in mm y^{-1}) for all samples and profiles.

	Uniform profile		Profile on top of gravel layer	
Soil	Pure	Amended	Pure	Amended
A	436	380	192	164
B	444	372	196	172
C	460	402	212	192
D	472	440	240	212
E	504	476	320	248

From this table two conclusions can be drawn. First, the amendment of 10 Vol. % organic matter decreases the irrigation demands significantly for both types of profiles.

Secondly, a 30 cm thick profile on top of a gravel layer reduces irrigation requirements by almost 50% compared to a uniform profile, at least for this 6% dry year 1994. This is also visible in Figure 5.11, where the transpiration reduction is presented for the year 1996 for all samples.

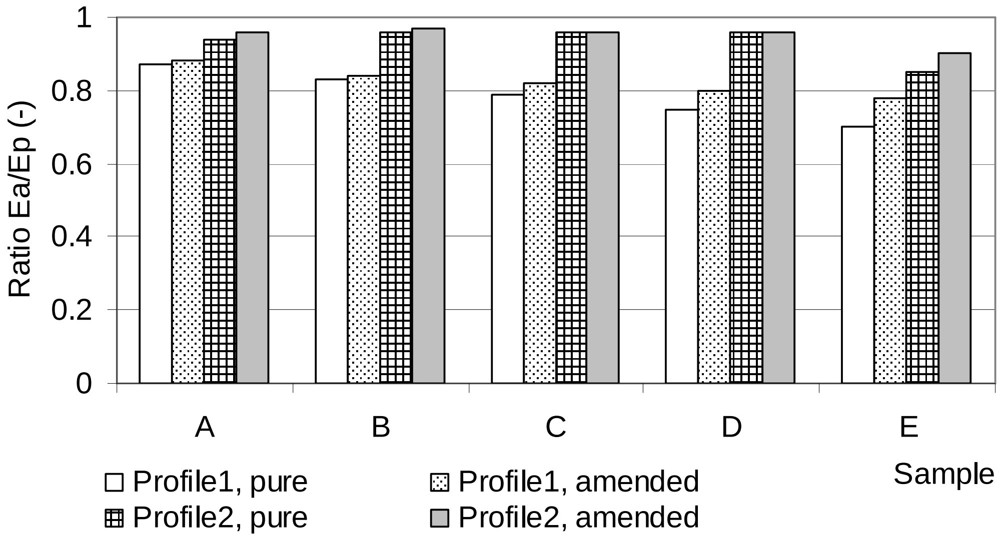


Figure 5.11 The average transpiration ratio of all profiles and samples over the year 1996.

In general the average transpiration ratio decreases from fine-textured to coarse-textured. Amending organic matter increases the transpiration ratio, so does the presence of a gravel layer. Figure 5.12 shows that amending organic matter to the soil decreases the amount of water flowing through the bottom of the soil profile. This figure also shows average fluxes of all samples and profiles used in this study. Generally, the profile with the gravel layer shows a decrease in the bottom flux compared to the deep profile.

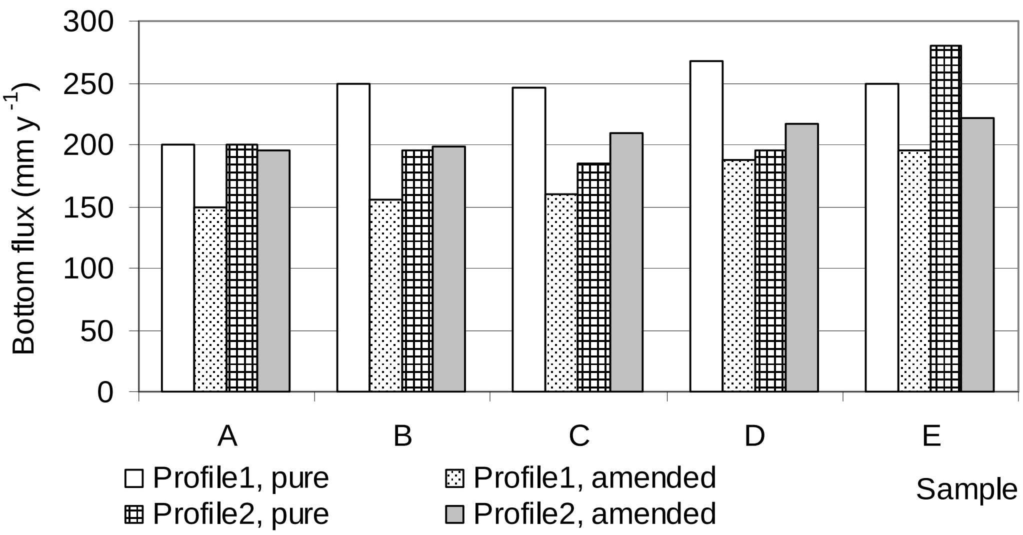


Figure 5.12 The flux (mm y^{-1}) through the bottom of the top layer for all profiles and samples.

5.4 Conclusions

- The dataset gathered in this study increases the understanding of the hydrological behavior of coarse soils, although additional research is needed to better understand the processes in coarse soils near saturation.
- Furthermore, the innovative polymer tensiometers (Van der Ploeg et al., 2008) could be used instead of the ceramic ones to better understand the hydraulic processes in dry soils. These tensiometers have a far larger measuring range than the standard ceramic tensiometers, and only fail at pressure heads below -20.000 cm.
- For the sand mixtures used in this study, we observed a significant effect of texture and organic matter addition on hydraulic properties. Saturated hydraulic conductivity increased with coarser texture, while for pressure heads smaller than -50 cm unsaturated hydraulic conductivity decreased with coarser texture. Also water retention capacity and the amount of plant available water decreased with coarser texture. Addition of 10 vol. % organic matter considerably reduced the

effect of texture on hydraulic properties. It reduced saturated hydraulic conductivity with one to two orders of magnitude, increased unsaturated hydraulic conductivity for pressure heads smaller than -50 cm, and increased water retention capacity. For the amended textures the amount of readily available water increased between 144% (sample B) to 434% (sample E) compared with the pure, mineral samples. This complies with the experimental results of McCoy et al. (2007).

- The coarse-textured pure soils we studied fall into the USGA specifications for constructing putting greens. Results indicate that these mixtures can contain only 2 to 16% plant available water and therefore need frequent irrigation to maintain plant growth possibilities. Addition of organic matter seems a good solution to reduce the irrigation water requirements, but increases the risk of runoff because it dramatically reduces K_{sat}. In the current study, the saturated hydraulic conductivity dropped below the value recommended by the USGA (3.6 m d^{-1}).
- The ratio between actual and potential plant evaporation is higher in case a gravel layer is used below the rooting zone compared with a uniform profile. This is due to the fact that water only flows into the gravel layer when the pressure head at the layer interface exceeds a certain limit.
- Adding 10 vol. % of organic material will decrease the amount of required irrigation water and thus will help to reduce the outflow of solutes and nutrients from the soil profile also.

6 Irrigation of a golf course in the southern part of The Netherlands: simulation versus practice

On one of the greens of a golf course in The Netherlands, soil physical properties have been determined, and rainfall, irrigation applications, and soil water contents measured during a one-year period. The numerical model SoWaM has been applied to compute the moisture content changes in time, and these show a good agreement with obtained measurements. Thereafter, the calibrated model has been used to compare computed versus actually applied irrigation quantities and timing. Results indicated that computed and applied irrigation amounts were almost equal on a yearly basis, however the days of irrigation differed. Basically, the greenkeeper irrigated less during the first phase of the growing season, while later on sometimes over-irrigation took place when there was no real need.

Adapted from

Wesseling, J.G. , C.J. Ritsema, K. Oostindie, C.R. Stoof and L.W. Dekker.2009. A new, flexible and widely applicable software package for the simulation of one-dimensional moisture flow: SoWaM. Submitted to Environmental Software and Modelling.

6.1 Introduction

The software package SoWaM (Wesseling et al., 2009c) was applied to investigate the irrigation water requirement of the 18-hole golf course Toxandria, located in the southern part of The Netherlands. The golf course has 17.5 ha of playable turf, of which approximately 1 ha is in use as greens. Water use for the greens of the golf course was recorded in time by the greenkeeper. From these data, the amounts of irrigation applied for the year 2004 could be derived. In 2005 a set of TDR-sensors was installed in a green at several depths. The moisture content values were measured by these sensors at regular time intervals and were stored by a datalogger. The memory of the datalogger was emptied every 15 minutes through a GPRS connection. The moisture content values obtained in this way were stored in a database. A linked web-page was developed to enable visualization of the moisture contents on a continuous basis.

6.2 Materials and methods

Soil samples were taken on one of the greens of the golf course for determining the soil physical characteristics (see Figure 6.1). These samples were analyzed in the soil physical laboratory of Alterra using the constant head method and Wind’s evaporation method (Halbertsma and Veerman, 1994; Stolte and Veerman, 1990; Wind, 1966). A series of cubical splines (Wesseling et al., 2008b) was fitted through the measured values yielding the soil moisture retention curve and the unsaturated hydraulic conductivity of each sample (Figure 6.2). Similar data were obtained for the subsoil of the green under study. Meteorological data (precipitation and evaporation) for the location of the golf course were obtained from a meteorological service in The Netherlands. Soil moisture flow was simulated with the SoWaM software package (Wesseling et al., 2009c).

Figure 6.1 Taking soil samples at the green of the golf course.

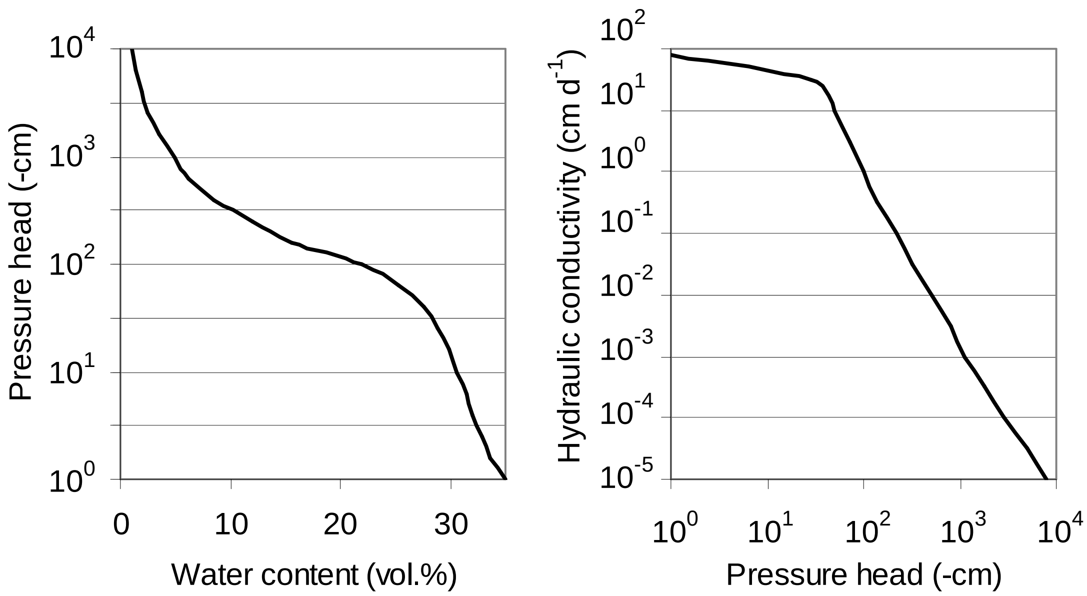


Figure 6.2 Soil physical characteristics of the topsoil of one of the greens on the Toxandria golf course.

6.3 Results and discussion

The irrigation trigger value was calibrated by comparing measured and computed soil moisture contents for the second half of 2005. Per irrigation event, 3 mm of water was supplied, the greenkeepers standard irrigation supply. The best results were obtained with an irrigation trigger at a transpiration ratio of 0.95. The measured and computed moisture contents of the green at 5 cm depth are presented in Figure 6.3. In general the computed and measured moisture contents agree rather well, except in the wet periods where the computed moisture contents are higher than the measured ones.

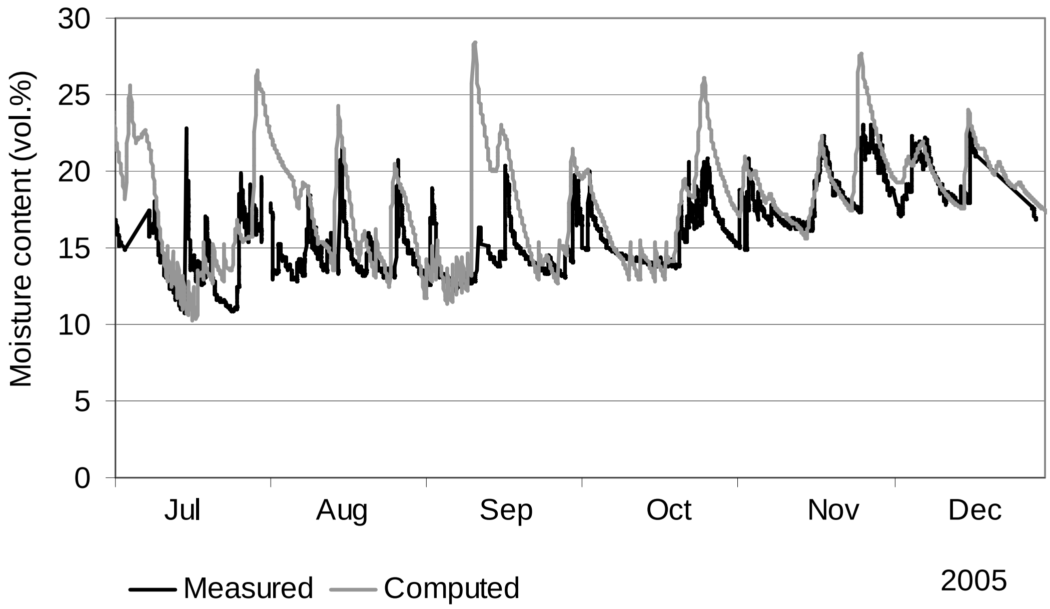


Figure 6.3 Computed (grey) and measured (black) moisture contents at 5 cm depth in one of the greens of golfcourse Toxandria during the second half of 2005.

Hereafter, the SoWaM simulation model has been used to compute the irrigation needs of 2004 with the irrigation trigger described in the previous paragraph. Actual irrigation dates of the greenkeeper, the ones computed by the model, and the measured precipitation are presented in Figure 6.4.

Figure 6.5 shows the actually applied and computed dates of irrigation for the year 2004. In total, the greenkeeper irrigated 168 mm in 56 applications between April 1st and the end of October, and the model 180 mm in 60 applications.

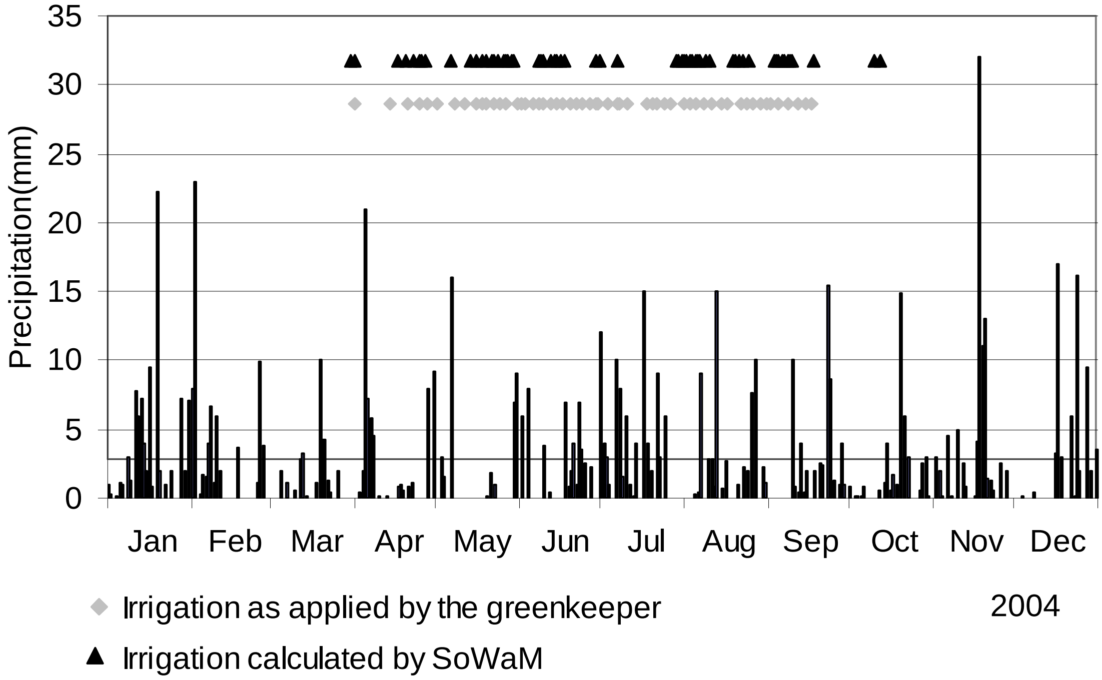


Figure 6.4 Measured precipitation, irrigation applied by the greenkeeper and computed irrigation by the SoWaMCalc model.

Figure 6.5 indicates further that the model irrigates slightly more in the early growing season between the beginning of April and the beginning of July. According to the model, it was not necessary to irrigate between the beginning and the end of July, though the greenkeeper still irrigated in this period on a regular basis. In addition, from early April until June 18th, the model indicated 29 days where irrigation would have been required. In the same period, the greenkeeper irrigated only 23 times. In the following period (through July 29th) it is relatively wet and the model only indicates 4 irrigation days, while the greenkeeper irrigated 15 times, which basically leads to unnecessary water use. This indicates that such model applications, when done realtime, can be used by the greenkeepers to improve irrigation scheduling on their golf courses. This might help to reduce irrigation water quantities and prevent unnecessary losses to underlying groundwater systems.

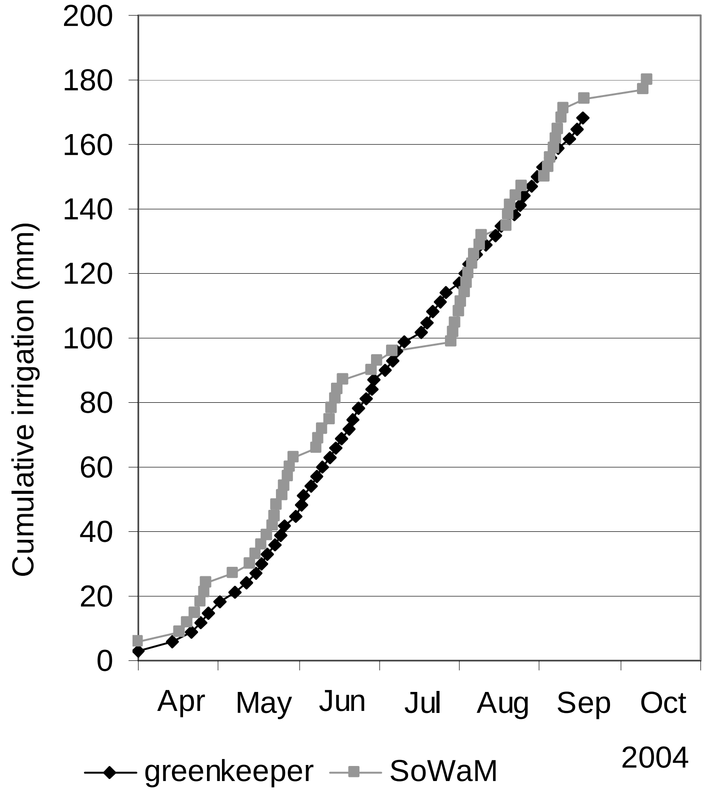


Figure 6.5 Cumulative irrigation applied by the greenkeeper and computed irrigation by the SoWaMCalc model.

In this example the irrigation criterion has been calibrated on the greenkeeper's irrigation scheduling, which was validated for a different period. Another possible application is to apply the knowledge of the grass scientists about situations at which turf damage will occur and use this knowledge as a trigger for irrigation. This might help also to potentially prevent losses of nutrients and the development of dry spots on turf (Dekker et al., 2004; Dekker et al., 2005; Ritsema et al., 2004).

6.4 Conclusion

This case study showed a possible application of SoWaM as a tool to determine and evaluate the irrigation requirements of a golf course. In combination with the expert judgement of an experienced greenkeeper, real-time application of a simulation model can lead to improved irrigation scheduling, potential savings in water consumption, better turf quality and reduction of associated energy costs. Extending the SoWaM simulation model with a solute and/or plant nutrition module could yield a helpful tool from this perspective.

7 Animating measured precipitation and soil moisture data

Nowadays more and more measurement sites are installed in the field to gain insight in the process of 2-dimensional moisture flow in soils, in dependence of the weather conditions. As these measurements often yield a large amount of data, visualization can be helpful and therefore a software package was developed consisting of several tools to process the measured data by creating animated movies of the changes in soil moisture content in time. This Chapter presents the software, the dataflow between the tools, a description of the tools and some examples of in- and output.

Adapted from

Wesseling, J.G., K.Oostindie, L.W. Dekker, E. van den Elsen and C.J. Ritsema. 2008. Animating measured precipitation and soil moisture data. Computers & Geosciences 34: 658-666.

7.1 Introduction

Soil moisture flow is a complicated process that often shows a large spatial and temporal variation. Numerical models are available to simulate 1 dimensional flow, e.g. SWAP (Kroes and van Dam, 2003; Kroes et al., 2008; Van Dam et al., 2008), Daisy (Hansen et al., 1990), Hydrus1d (Simunek et al., 1998) and SoWaM (Wesseling et al., 2009c), 2-dimensional flow (Vogel, 1997; Heinen, 1997; Simunek et al., 1999) and 3-dimenaional flow (Russo et al., 1998). The website of the International Groundwater Modelling Centre (http://www.mines.edu/igwmc/software/) presents an excellent overview of all models and their availability. Despite the improvement of numerical models, field measurements remain of great importance for researchers. The reasons are twofold: i) numerical models need calibration and validation and ii) field measurements help to gain new insights in physical processes affecting water flow, such as soil layering, water repellency and swelling and shrinking processes. As electronic measuring devices nowadays are becoming cheaper and more sophisticated, soil moisture content is now often been measured at a high spatial and temporal resolution. For instance, sensors based upon the TDR (Time-Domain Reflectometry) principle (Baker and Hillel, 1990; Heimovaara and Bouten, 1990; Topp et al., 1980; Van den Elsen et al., 1995) can be used for this purpose. Measured values are either stored on a datalogger or some computer, and generally data processing takes place at the office.

In the Soil Science Centre of Wageningen University and Research Centre, detailed field investigations on flow in soils takes place at several sites within The Netherlands. In order to account for spatial heterogeneity, numerous sensors are installed at short distances. For an example see Figure 7.1 where a grid was created of 40 sensors (10 horizontal positions x 4 depths in a vertical transect of 1 m long and 30 cm deep), while another identical grid of sensors was installed at some distance from the first one to study the effects of different soil treatments.

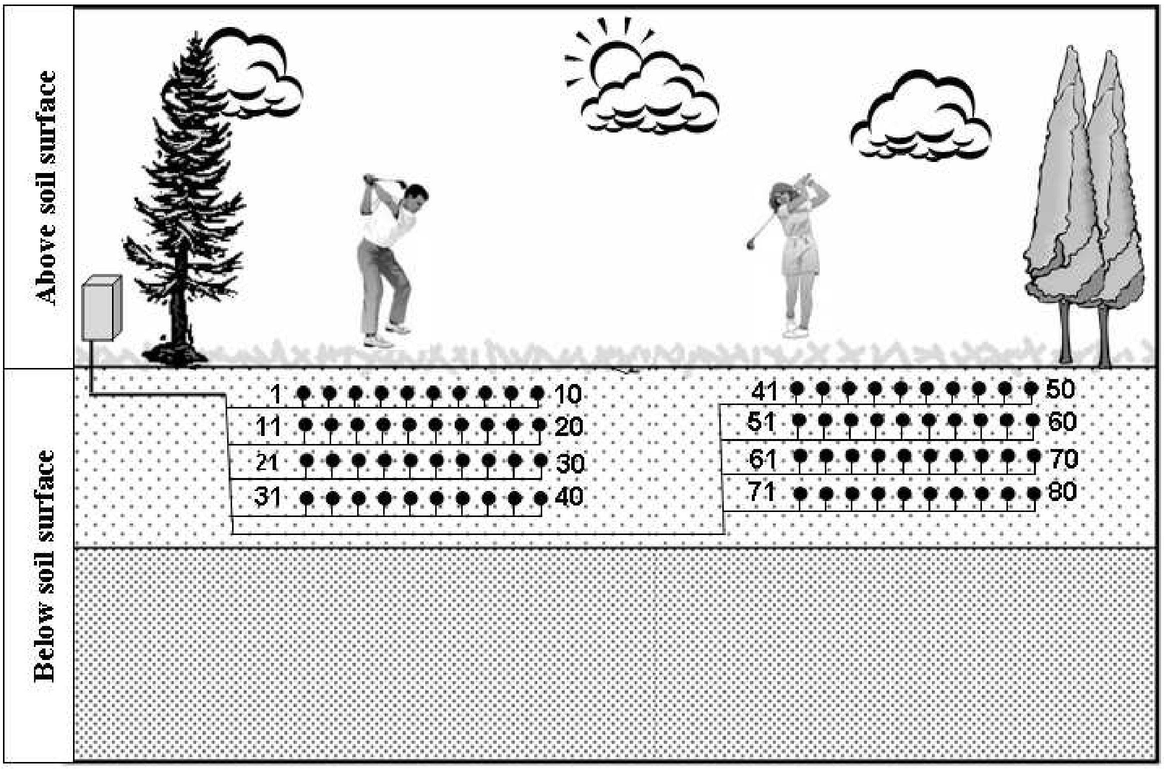


Figure 7.1 Schematic representation of a measuring site. To investigate the influence of different treatments, two sets of sensors have been installed.

Results of field studies have amongst others been published by Oostindie et al. (2005a; 2005b).

7.2 Processing the data

7.2.1 General

At first the measured moisture contents and, if available, also drain outflow data, were processed and visualized by copying the data-files into an Excel spreadsheet. The data was checked manually and graphs were made automatically. In the following paragraphs we shall show how a combination of two Excel-spreadsheets (with some Visual Basic code) and a Delphi program can speed-up the data processing and create animations and slideshows of spatially distributed measured values automatically (Wesseling et al., 2008a). The Excel file RainProcessor contains a small VB-macro that reads the input files with measured precipitation data, puts the data in the correct order, calculates intensities and shows the data in monthly graphs. TDRProcessor is an

Excel file to read the measured moisture contents, sort them, write the data in a specified way and make line-graphs of the data. The program TDRProcessor.exe then reads the four Excel files (outflow1.xls and outflow2.xls containing data on drainage outflow, tdrprocessor.xls containing TDR data, and rainprocessor.xls containing precipitation), creates 2-dimensional contour plots of the measured moisture contents and shows the precipitation and drain outflow in time.

7.2.2 Dataflow

Before showing the animated precipitation and moisture content changes in time with the program TDR-processor, the appropriate data should be processed by and stored in the Excel files. The order in which these data are processed is not important, as long as they are available before starting the animation program. This process is shown in the flowchart of Figure 7.2.

7.2.3 Precipitation

Precipitation is usually measured with automatic gauges. A signal is given after a certain amount of precipitation (e.g. 0.2 mm) has fallen. The built-in software of the automatic gauge records the time at which the signal was recorded and adds the amount of precipitation to its memory. This way the file with precipitation data will consist of lines with only three items: a date, a time and a cumulative precipitation. After the data has been read from the gauge, the memory will be reset and cumulative precipitation will start from zero again. To process the precipitation data, the Excel-file RainProcessor.xls should be loaded into Excel. After opening this file, 13 worksheets will be available: one control-sheet and 12 worksheets which contain data for one month each. The worksheet 'Control' is the one where you give some details about the files to read and where you can start the data processing. All files with precipitation from the meteorological station should be stored in one single directory first. The first characters of the names of the files with precipitation data should be the same, representing the name of the station. Pressing the ‘Show’-button will start a VB-macro for reading and processing the data files. When processing is finished every month-

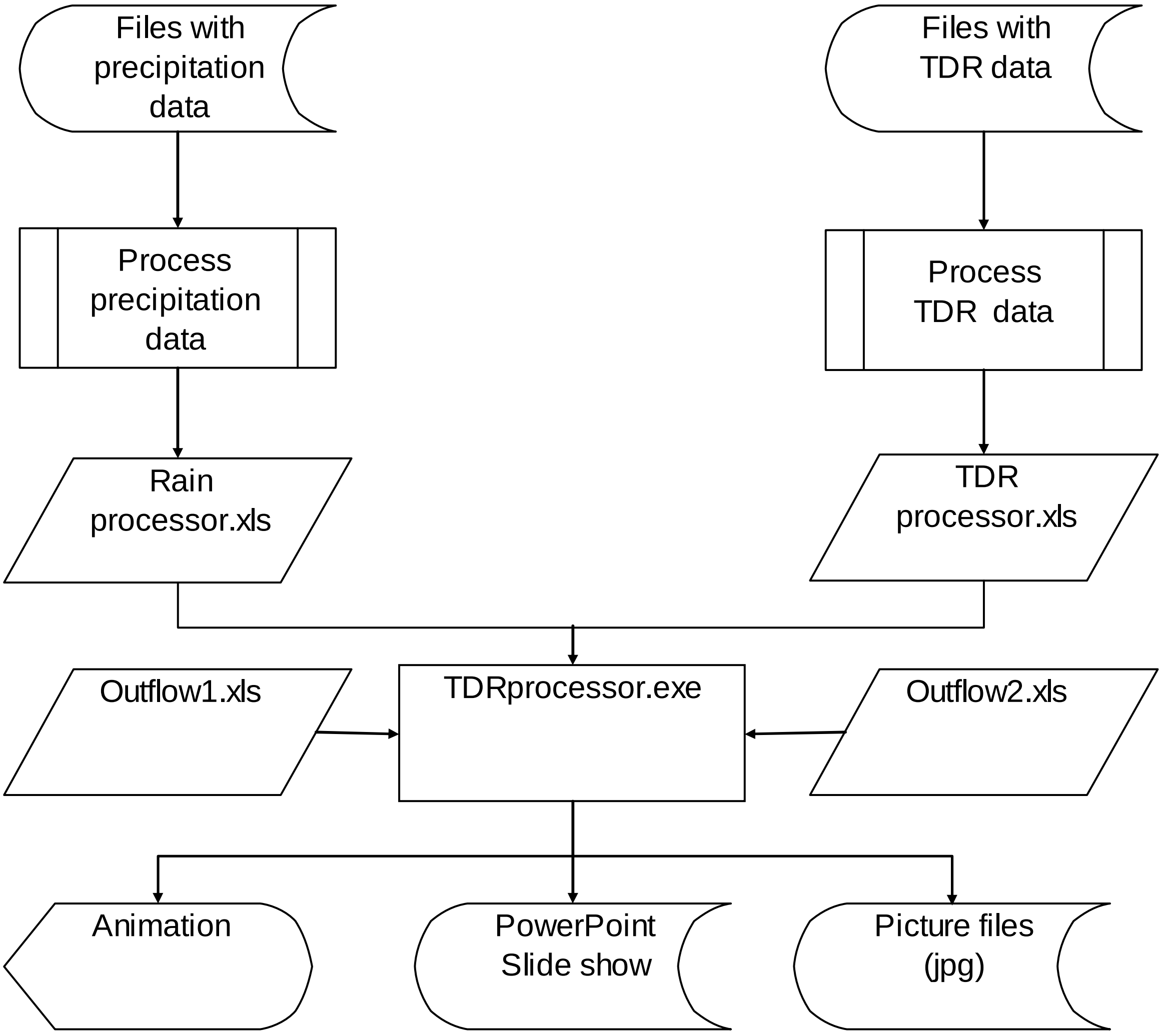


Figure 7.2 Flowchart for processing precipitation-, drain outflow- and TDR-data.

sheet contains three columns with data: the date-time, the cumulative precipitation (mm) and the calculated intensities. These data are shown graphically as presented in Figure 7.3.

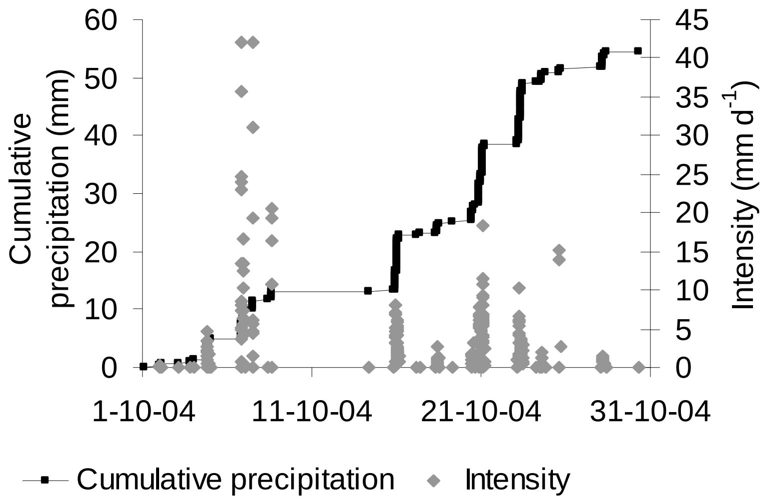


Figure 7.3 Example of recorded cumulative precipitation and rainfall intensities.

7.2.4 Moisture content

Usually the interval between measurements of the TDR-sensors varies between say 10 minutes up to several hours, depending on the interest of the researcher. The TDR sensors are distributed over a number of different fields ('plots'). Each plot can have different properties (e.g. plot 1 is untreated, plot 2 has been treated with product A, plot 3 with product B, etc.). The sensors are read one-by-one by the registration unit. This implies there is a small time-difference between the registrations. The registrations will be copied from the registration unit to a file. Each line of the file contains a lot of information, including the sensor number, the date, the time and the measured moisture content.

To process the data measured with the TDR-sensors, the Excel-workbook TDRProcessor.xls has been developed. The current version of this tool is able to handle data of 5 different plots and up to 10 sensor rows (depths) per plot. After opening the workbook, a lot of worksheets become visible. These are presented in Table 7.1

Table 7.1 Worksheets in Excel-application TDRProcessor.

Sheet	Contents
Control	File processing, distribution of sensors over plots, data processing
AnimaControl	X- and Z-positions of the sensors
Colors	Color-settings of the animation
Moisture	The moisture contents
Ka	The rough measurement data
Plot1	Graphs with moisture content of plot 1
Plot2	Graphs with moisture content of plot 2
Plot3	Graphs with moisture content of plot 3
Plot4	Graphs with moisture content of plot 4
Plot5	Graphs with moisture content of plot 5
Averages	Averaged moisture contents at one depth for each plot
PlotAverages	Plot with average moisture contents.

Worksheet 'Control' (Figure 7.4) is the main worksheet. Cells A1 and A2 should contain the directory of the data-file to be processed and the name of the data file respectively. Pressing the button 'Add file' causes the program to read the data from the file and put them into the worksheets 'Moisture' and 'Ka' from where they will be read by the animation program. Pressing the 'Show'-button causes the data on the worksheet 'Moisture' to be processed and graphs to be made for every plot, including averages. Worksheet 'AnimaControl' is meant to provide data to the animation program TDRProcessor.exe. It contains the positions of all sensors for the first plot. (Take care that the z-values of the sensor-positions are either increasing (positive) with depth or decreasing (negative) with depth. The program does not have any checks built-in for the correctness of coordinates).

It is assumed that the other plots have the same sensor-coordinates. See (Wesseling, 2007) for more details. The animation program presents the moisture contents by different colors. This means a number of moisture content classes have to be defined beforehand. Each class is assigned a minimum value, a maximum value and a different color. Therefore the worksheet 'Colors' (Wesseling, 2007) is introduced to enable the users to define their own classes and corresponding colors for the animation. The colors have to be entered as RGB-values.

Figure 7.4 Main worksheet ('Control') of workbook TDRProcessor.

The worksheets 'Moisture' and 'Ka' contain the measured values. In ‘Ka’ the measured di-electric value is shown from which the moisture content in ‘Moisture’ is calculated by the measuring device (Wesseling, 2007). Every column represents one sensor except the first column where the date and time of measurement are written. At each of the worksheets 'Plot1', ..., 'Plot5' the moisture contents are shown at each depth.

The worksheet 'Averages' contains moisture content data averaged over one depth. This worksheet is meant only as an intermediate for 'PlotAverages' (Figure 7.5) which contains charts. Every sensor depth has its own chart where each line represents a plot.

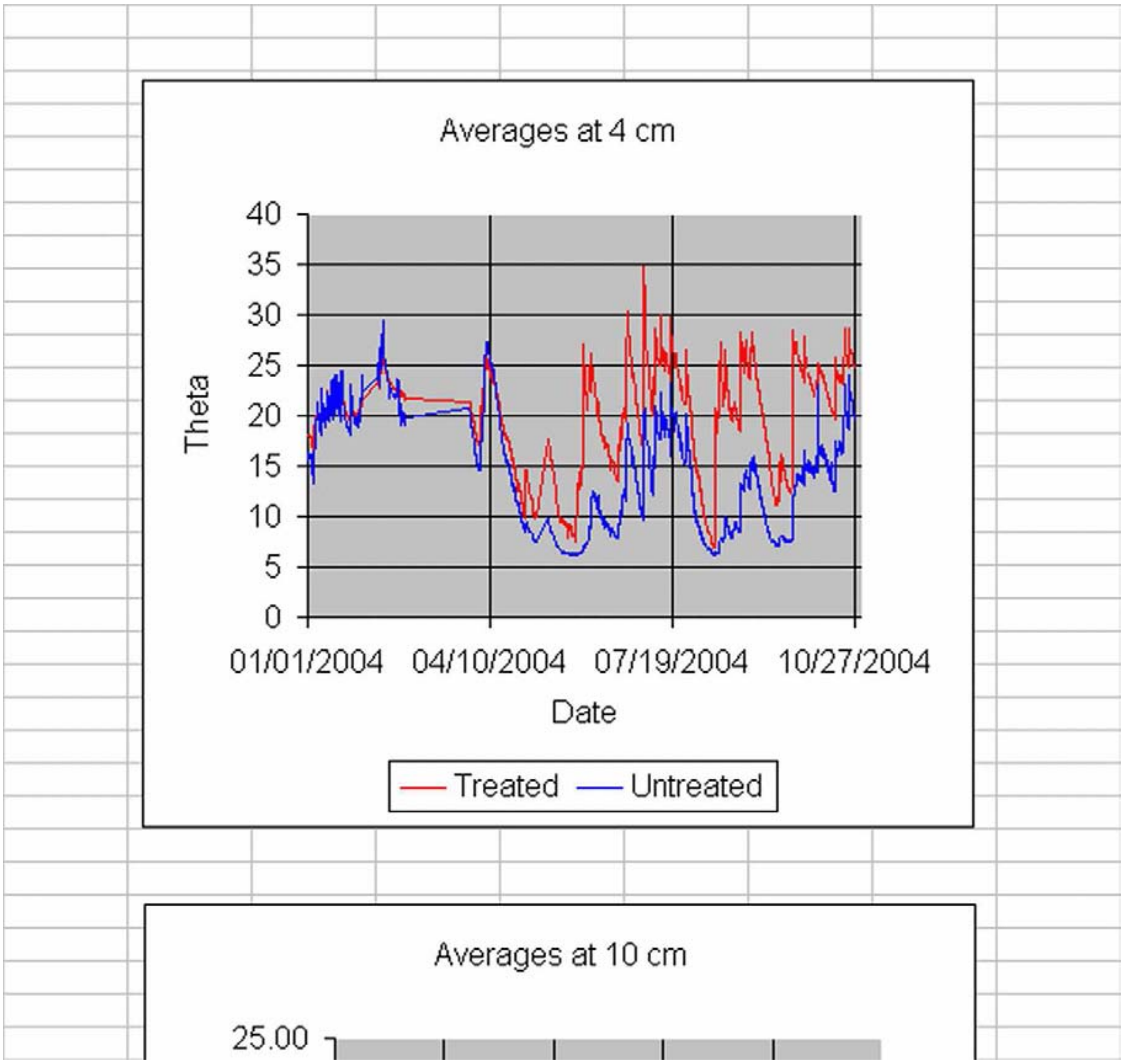


Figure 7.5 Part of worksheet with averaged moisture contents per plot. Please note that in the period between 2 and 4 October measurements failed for a while, yielding straight lines in the graph.

7.3 Creating animations

In the previous sections of this chapter we described the preparation of data to be used in the animation software package. The TDRProcessor.exe tool is able to visualize changes in soil moisture contents and precipitation for 1 plot or 2 plots at the same time. Before starting the animations, the first and last date of animation should be selected by choosing the appropriate dates on the calendars (Figure 7.6).

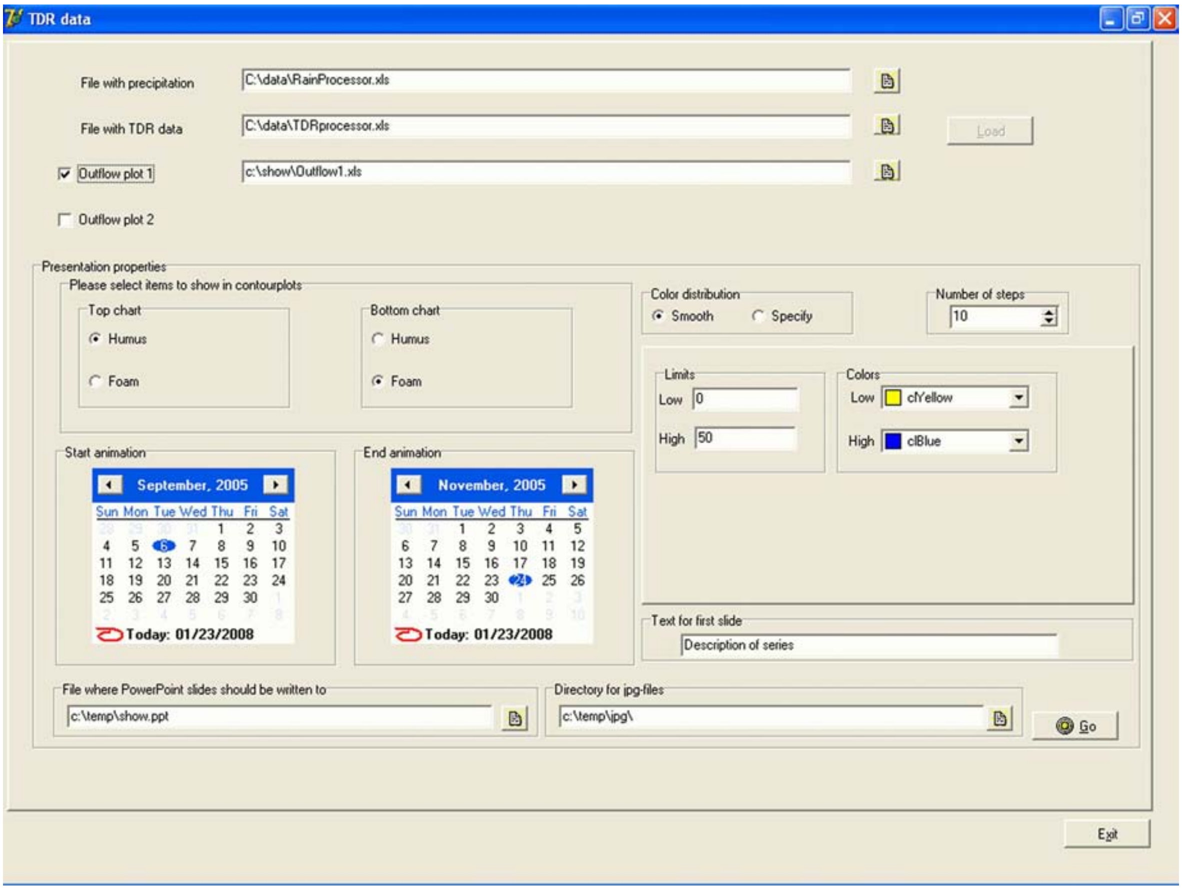


Figure 7.6 Control screen of program TDRProcessor after reading data-files.

The number of soil moisture classes (and thus the number of colors) may vary between 2 and 50, but normally around 4 to 8 classes are sufficient to achieve good animation results. Within the TDRProcessor software, two color distribution methods are available: a smooth distribution and a specific distribution. In case of a smooth distribution you can enter the minimum and maximum value of the moisture content (in %) you want to show. Below these minimum and maximum values you can select the corresponding colors. If you select the specific distribution, you should specify the low- and high value for each interval, as well as its color.

The color can be entered as a RBG-value (Figure 7.7). Pressing the button on the right-hand side of the color selection panel causes a color selection screen to pop up. To create this form, the freeware component MCColorPanel (developed by Leonid 'MC' Belousov, see www.mastercluster.com) was downloaded and installed.

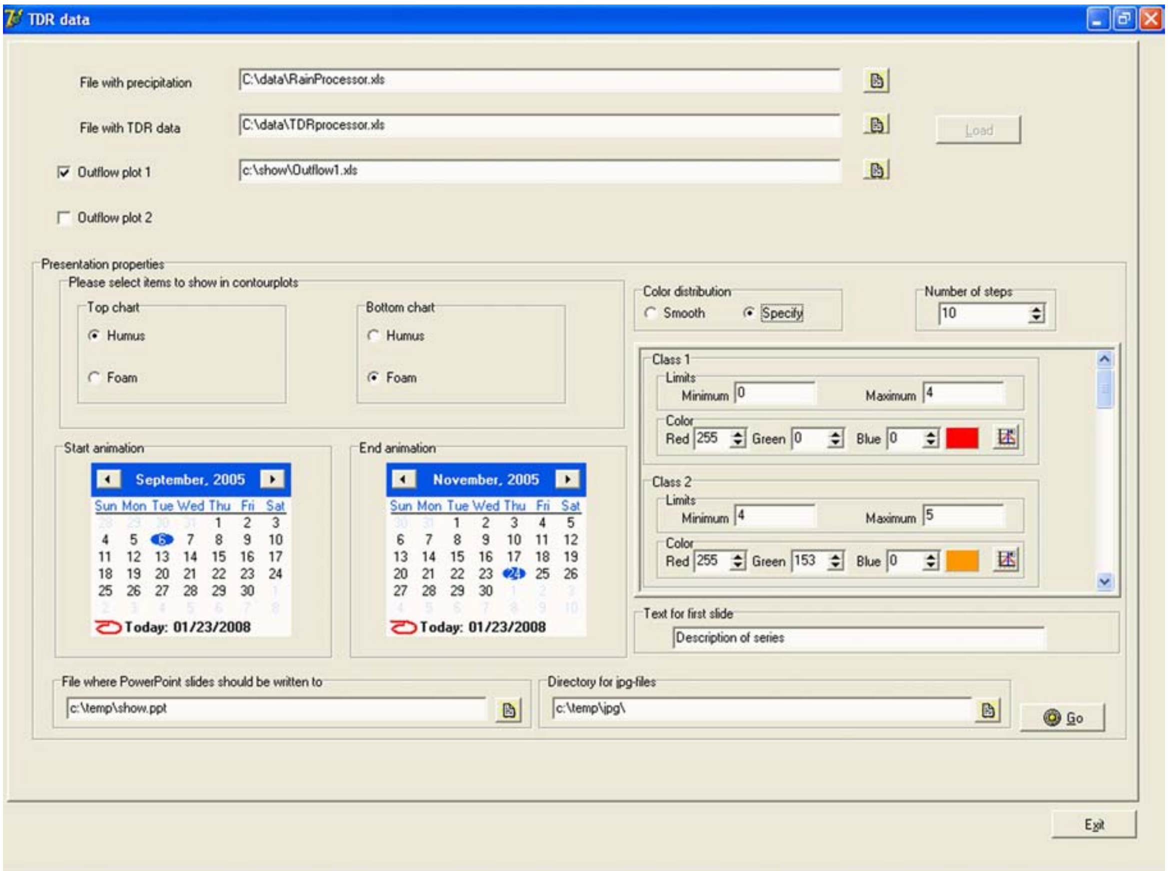


Figure 7.7 Control screen when colors for different moisture classes are specified.

The initial colors are loaded from the sheet 'Colors' of the spreadsheet with TDR-data and stored there again when animation starts. Clicking the 'Go'-button will cause the next page to appear (Figure 7.8). The top graph represents the precipitation data. The middle and bottom graphs are designed to show the contour graphs of the data you selected. It is possible to change the speed of the animation by changing the position of the slide-rule at the bottom of the form.

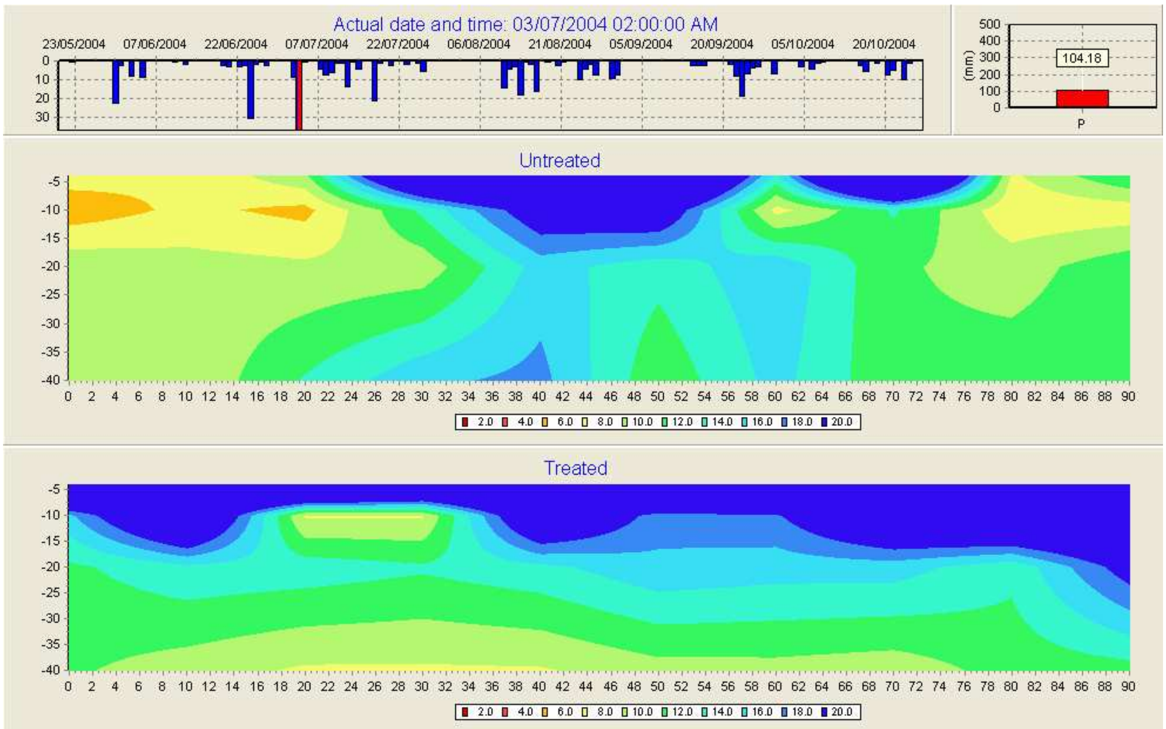


Figure 7.8 Form with graphics during animation.

During animation a red line will move through the precipitation chart to indicate the date for which the contour-plots are actualized. As the precipitation is presented as daily totals, sometimes it may happen that the moisture content of the plots increases only at the end of the day, even though the precipitation chart indicates precipitation. In this case the precipitation actually took place at the end of the day when also the TDR-sensors are responding. At the top of the upper contour-plot the date and time are presented as well. After pressing 'Pause' you can either resume the animation (by pressing the same button once more) or press 'Step' to manually move forward in time.

Whenever you are in the 'Pause'-mode, you can copy the charts to the clipboard. The three graphs will then be put together on the clipboard from where you can paste them into an application like PaintShop, Word, Powerpoint etc. Figure 7.9 presents the graphs of an animation of measurements on an experimental slope.

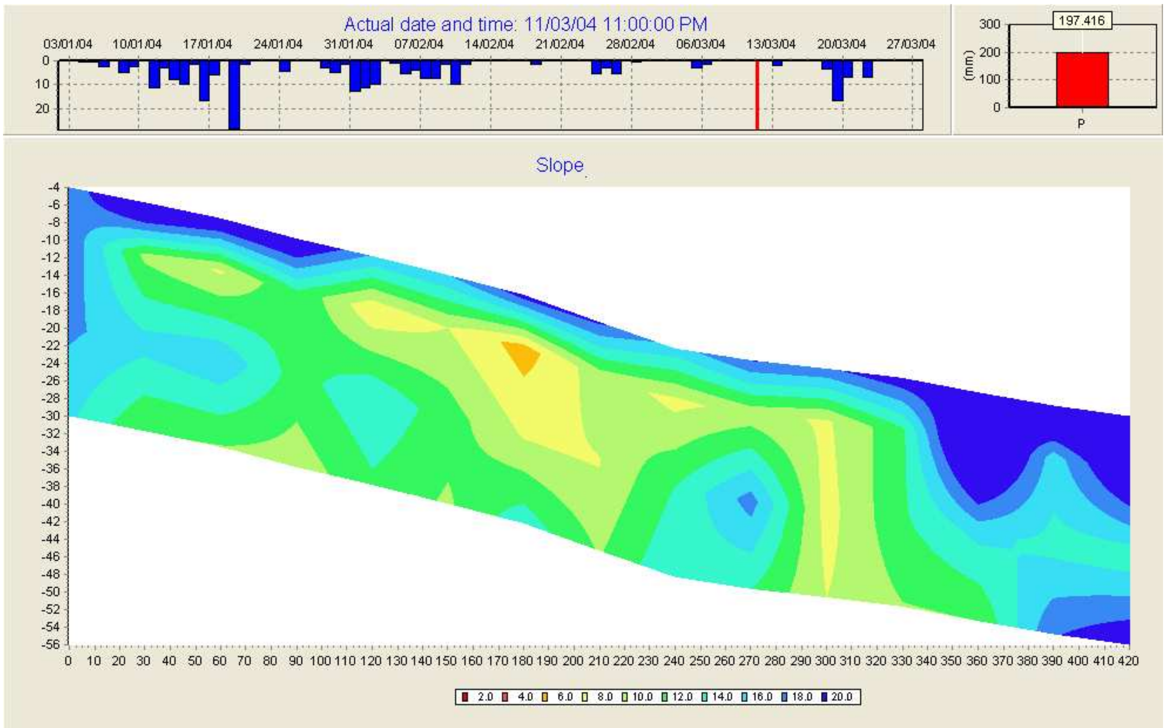


Figure 7.9 Example of graphs as copied to the clipboard.

In Figure 7.10 a series of measurements results are shown before, during and at the end of a rain event. It clearly shows that water initially infiltrated mainly at the top and bottom of the slope and that less infiltration took place in between.

7.4 Final remarks

- The program stores the jpg-files as Fxxxxx.jpg where xxxxx is a number. There is no check on existing files, so one should remove old files from the output directory of the animation program yourself before starting a new animation.
- Separating the data-preparation and visualization from the animation itself has the advantage that the benefits of Excel and Delphi are used. Writing it all in Excel / VBA would make it slower and less sophisticated in relation to the 2-dimensional graphical design.

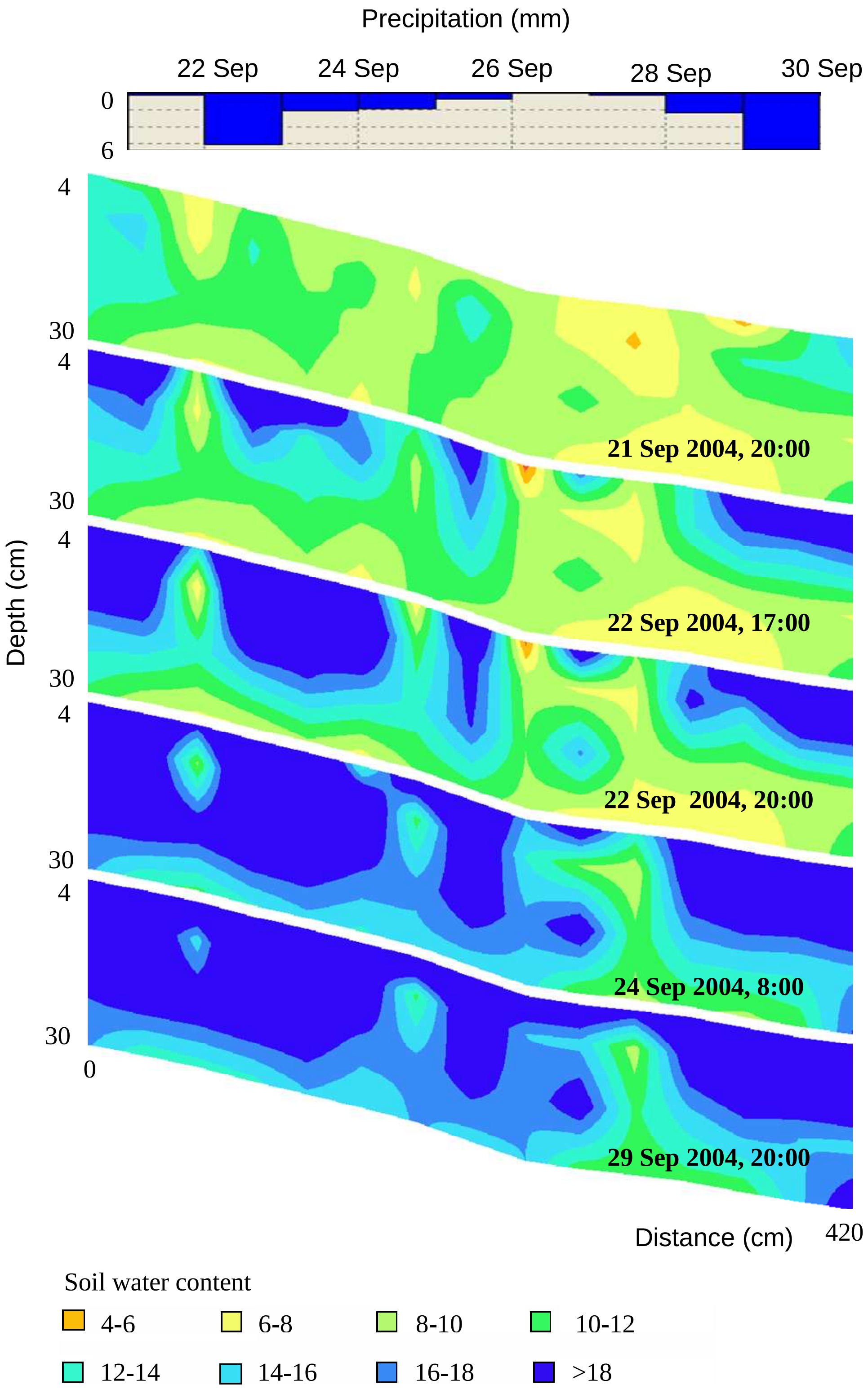


Figure 7.10. Moisture content distributions on an experimental slope before, during and after a period with precipitation.

- Applications of this program are not limited to soil moisture. For instance, soil temperatures or solute concentrations can be visualized as well, or any other property, as long it has been measured in 2 dimensions.
- The developed software can be used for visualizing the output of numerical simulation models as well.
- Animations prepared with the newly designed software have been shown to audiences at international congresses and conferences already.

8 Synthesis

8.1 Achieved results

The main objectives of this study were: to describe soil physical functions in a mathematically more accurate way, to investigate the soundness of the Staring Series soil physical database, to develop and apply a new 1-D soil moisture flow simulation model and to expand the Staring Series with data on coarse textured soils. All these objectives have been addressed through a series of interrelated research activities, comprising a mixture of laboratory investigations, field monitoring campaigns and modeling work. The main activities executed during this PhD study and obtained results are the following:

- *Describing the soil physical relationships in a mathematically more accurate way*

The soil water retention function and hydraulic characteristics are generally described using the Mualem - Van Genuchten equations. In that approach, the Mualem - Van Genuchten equations are fitted through a series of measured points to obtain the related equation parameter values. However, so far it is not always possible to fit these equations through the measured data with sufficient accuracy. Therefore in Chapter 2, a cubical splines method using a Mean Distance from Point to Line (MDPL) object function has been introduced and tested on several sets of soil moisture retention and hydraulic conductivity data. It appears that the MDPL method significantly increases overall fitting results compared with other approaches currently known and in use.

- *Investigating the validity of clustering data from soil samples into soil physical classes*

The way the well-known Staring Series has been designed originally aimed to categorize soil samples into soil physical classes based on textural information, and to derive “averaged” soil physical properties for these classes. A detailed analysis has been performed regarding the soundness of this approach in order to unravel if different soil physical classes within the Staring Series reveal statistically different outcomes from a hydrological point of view when used for modeling purposes. Results presented in Chapter 3 indicate that samples grouped into a single Staring Series class not necessarily show identical hydrological responses. Furthermore, no statistical significant differences in hydrological output could be found between most of the distinguished Staring Series classes either, indicating that grouping of samples should be done according to other criteria than soil texture and organic matter content alone.

- *Model development*

Current available simulation models to describe soil moisture flow in the unsaturated and saturated zone are all different and not always exhibit the features which one preferably needs for a specific application or study. Therefore, within the context of this thesis, a new software package (SoWaM – Soil Water Management) was developed capable of simulating 1-D soil moisture flow with sufficient complexity, the possibility to describe soil physical relationships using the cubical splines method as described in Chapter 2, the use of variable (including extremely small) time steps, and the possibility to store and present model output efficiently and graphically. The software package consists of a MySQL database and a number of executables. Furthermore, several additional features are implemented in the model, like automated irrigation control, use of different types of irrigation criteria, and breakthrough of water to underlying coarse layers when a certain pressure head is reached at the layer interface.

- *Determining soil physical properties of coarse textured mixture*

So far, only little information could be found on soil physical properties of coarse textured soils. Also, no information could be found in the widely used Staring Series database. Therefore, the physical properties of a series of artificially created coarse sand mixtures were determined in the laboratory using the constant-head method and Wind’s evaporation method, respectively. Thereafter, the hydrological behavior of these coarse sand mixtures was studied using the newly developed SoWaM model. Results as described in Chapter 5 indicate significant hydrological differences between the samples in dependence of the grain size distributions used (in preparing the samples), as well as possible additions of organic matter. When used as rootzone mixtures for constructing golf greens, these different samples show distinct differences in irrigation water requirements. Also it is shown that less irrigation water is needed when instead of a homogeneous soil profile, a gravel layer is positioned directly below the rooting zone.

- *Computing irrigation requirements of golf greens*

In Chapter 6, the newly developed SoWaM model has been used for optimizing irrigation scheduling on the greens of a golf course in the southern part of The Netherlands. For that purpose, the soil physical properties of the rootzone layers have been determined in the laboratory, and additionally in-situ soil water contents have been measured in the profile at 15 minute time intervals. Information on precipitation and irrigation application were recorded too. Based on the obtained data, the SoWaM model has been calibrated, and thereafter used for comparing actually applied versus computed irrigation regimes. Results indicate slight differences only, with the numerical model showing more often irrigation during the early phase of the growing season, and less thereafter. However, yearly totals were more or less similar.

- *Visualizing measured moisture contents in two dimensions*

Currently, more and more detailed field investigations on soil moisture flow are taking place using advanced measuring techniques. Regularly, dense arrays of sensors are placed in vertical soil trenches to monitor soil water contents in two dimensions in high spatial and temporal resolution. Such monitoring campaigns reveal large datasets, which often can not be interpreted at once. For this purpose, a software package has been developed to visualize 2-D soil water content changes in time as animated movies. The software package has been tested and used for multiple datasets from the Netherlands and clearly show how water might move into soils. The software package distinctly helps in interpreting collected data in more detail and expand our current knowledge on flow processes through soils in general. Additional features of the software package are automated data processing, simultaneous visualization of time information and rainfall quantities, and the possibility to show more soil trenches on the screen at once.

8.2 Main conclusions

The main conclusions of this thesis are:

- Cubical splines using the Mean Distance between Point and Line criterion improves fitting results to measured soil physical data distinctly (Chapter 2).
- Distinguished soil physical classes in the Staring Series database do not necessarily differ hydrologically. An alternative classification system is required to group individual soil samples in unique soil physical classes, as using textural and organic matter content information alone is not sufficient for this purpose (Chapter 3).
- The SoWaM model is a highly flexible software package able to compute one-dimensional flow and transport in a spatially and temporally detailed manner using an open-source MySQL database for input and output storage. Additional features included are automated irrigation control, use of different types of irrigation criteria, and breakthrough of water to underlying coarse layers when a certain pressure head is reached above the layer interface (Chapter 4).
- Coarse textured mixtures behave differently from a hydrological point of view in dependence of the exact particle size distributions of the mixtures, as well as absence/presence of organic matter. Especially, when used for constructing putting greens on golf courses, slight differences in mixture composition might lead to large differences in irrigation water requirements (Chapter 5).
- Application of the newly developed SoWaM model to a golf course site in the Netherlands showed that irrigation scheduling can be improved, especially regarding timing of the irrigation water applications (Chapter 6).
- The newly developed visualization software package to process large datasets of measured soil water contents and rainfall data is helpful in interpreting obtained

data and the animated movies expand our knowledge regarding actual flow and transport mechanisms in soils (Chapter 7)

8.3 Discussion

8.3.1 Added value of the thesis

The research done and described in this thesis significantly advances the state of knowledge and provides added value through:

- Integrating research activities in the field and the laboratory with model development and application
- Addressing and linking different spatial scales, from the sample (cm) up to the 2-D soil trench scale (m)
- Enabling simulation of flow processes at variable time steps, ranging from milliseconds to days to properly account for water ponding processes, and potential runoff effects
- Providing a new fitting procedure to parameterize soil physical properties more accurately on basis of measured datasets, either derived in the laboratory or in the field
- Showing that the soil physical classes distinguished in the frequently used Staring Series not necessarily differ hydrologically, indicating that the Staring Series should be revised
- Adding information to the community on soil physical properties of coarse textured media, as relevant for several regions in the world, as well as for putting green construction
- Development and application of new user-friendly flexible model code for simulating 1-D soil moisture flow, describing processes currently not addressed in other comparable models
- Indicating that current irrigation practices on golf courses can be improved by using numerical models for irrigation scheduling, potentially leading to water

savings, better turf performance, less related costs, and a more sustainable environment

- Providing a software platform for visualizing large sets of soil water content and rainfall data by creating animated movies through time
- Recommending research needs to be addressed in the near future

8.3.2 Limitations of the study

Besides the above mentioned added value of this thesis, certain assumptions and decisions have been made as well which potentially limit the credibility and outreach of part of the obtained research results.

- First of all, during the execution of this Ph.D. study, direct use has been made of the Staring Series database without proper quality control of underlying information. It was assumed that a quality control had taken place in the past by researchers responsible for designing and constructing the Staring Series, however, at the end it appeared that this was done only partially and to a limited extent.
- A further critical analysis of the Staring Series data showed that soil physical properties have been determined in the past by a mixture of different measurement methods and techniques and applied by different researchers, basically making direct comparison between sample outcomes (even more) difficult.
- Despite that the newly developed 1-D SoWaM model code has quite some unique advantages, a wide-use of the model by others is not directly foreseen. As indicated earlier, many other simulation models exist, several far more advanced and with a longer development and application history. However, for the purpose of this PhD study none of these more advanced models provided the features which were finally included in the SoWaM model code.
- Soil physical properties have been determined for a series of predefined coarse textured mixtures manually prepared in the laboratory, and further evaluated hydrologically using the SoWaM model. Despite that useful information has been derived from this study, future activities should focus on coarse textured field soils

instead, and sample, determine and analyze these for further inclusion in the Staring Series and/or other databases.

- Despite that this thesis focuses on soil physical properties and model development and application, the scope of the study is still rather limited. Certain processes significantly affecting flow and transport processes in the field have not been taken into account or received insufficient attention due to limitations of time and resources. Especially, problems related to spatial heterogeneity (what is a representative sample?), time-variance of surface soils (what are the effects of land use and management?), weather effects (crusting, development of water repellency) and specific soil properties (swelling, shrinking, hysteresis) complicate flow and transport in real field conditions considerably, and will need appropriate attention in future research projects.

8.3.3 Potential institutional and policy implications

The research results described in this thesis might have potential institutional and policy implications.

First of all, it has been identified recently that the Staring Series are being used by many organisations in the Netherlands (and elsewhere) for a variety of reasons (De Vries et al., 2008). Among the users within the Netherlands are several Ministeries (LNV, VROM, V&W), DLG, MNP, Rijkswaterstaat, Provinces, Water Boards, research and educational organisations, consultancy firms, and organisations dealing with nature management. The Staring Series are used regularly as input for modeling studies to assess the risks of certain environmental threats, like pollution, soil compaction, organic matter loss, salinization and erosion, or alternatively to determine for instance crop productivity potentials or to evaluate possible effects of future water management strategies.

The wide range of applications of the Staring Series basically indicates that quality control of the database should receive the appropriate attention. The more important because results of modeling and scenario analysis are often used by policy makers for finetuning regulations or adapting strategies to reach certain policy and/or environmental goals.

Also in the light of the recently formulated European regulations on water (Water Framework Directive) and soil (Soil Thematic Strategy), availability and use of a sound soil physical database becomes increasingly more important. Fortunately, the Dutch Ministery of LNV provided substantial financial resources recently to further expand and professionalise the Dutch Soil Information System (BIS), of which the Staring Series is part also.

8.3.4 Research needs

Results of this thesis lead to the follow recommendations regarding the Staring Series soil physical database and how to proceed forward in the very near future:

- All available soil physical property data of the original Staring Series should be quality controlled using predefined criteria. Fortunately, this activity has been initiated since early 2008, and quality approved samples are stored in the so-called Priapus database from now onwards.
- Due to a current lack of quality assured samples, immediate actions should be undertaken to (re)sample all representative soil types in the Netherlands in order to create a thorough and sufficiently dense nation-wide database on soil physical property information.
- Precise procedures, protocols and harmonized methods should be defined for i) collecting soil samples in the field from the relevant soil types and soil horizons, ii) measuring the soil water retention characteristic, saturated conductivity, and unsaturated hydraulic conductivity function in a replicable and reliable way, preferably according to predefined ISO-standards, iii) processing obtained data in the laboratory to obtain the parameter sets of the Mualem – Van Genuchten equations or the parameters of the cubical splines approach as described in this thesis, and iv) data storage and a description covering information regarding

usability of the data and related limitations, including an accessibility platform for potential internal and external end-users.

- Due to the wide and frequent use of the Staring Series as shown by De Vries et al. (2008), the lack of quality control of earlier obtained data, and the potential far-reaching consequences of using the current soil physical database in modeling and scenario analysis, an urgent need exists for an immediate and substantial financial provision to arrive at a more trustable, sound, and scientifically based improved soil physical database covering all regions of the Netherlands.

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Summary

Chapter 1 describes the problems for which this thesis tried to find solutions. Accurate and reliable information of soil physical properties is of crucial importance when simulating transient unsaturated soil moisture flow and solute transport. These properties are either taken from existing databases or measured. Measured data, either obtained from the field or the laboratory, is often used to obtain the parameters of the Mualem – Van Genuchten equations. However, fits of the equations through the datasets, is achieved with variable success. A database for Dutch soils (the Staring Series) falls short in proving information on coarse sandy soils, restricting its applicability. The SoWaM model and spline interpolation of soil physical properties are applied to compare the irrigation regime of a numerical model with the one of an experienced greenkeeper. Furthermore, there is a lack of visualization techniques of the large number of data that is obtained nowadays with automatic monitoring in the field. Such visualization may help to interpret the regulating processes. All these emerging needs were brought together and addressed in this Ph.D-thesis.

Due to the problems with fitting the Mualem-Van Genuchten equations, a new and simple method to (mathematically) describe soil physical properties was developed using the spline approximation. In a cubical spline approximation, a function is described by a number of piecewise-continuous 3rd degree polynomials. The parameters of these splines are selected in such a way that the function and its derivatives are continuous functions. The mathematical theory of these splines and a simple optimization method (Controlled Random Search) have been explained in Chapter 2. The Mean Distance from Point to Line (MDPL) is introduced as the average distance between a measured point and the calculated line. Five different object functions are compared: the sum of deviations, the sum of squared deviations, the sum of the relative deviations between measured and calculated values, the ratio between measured and calculated values, and the MDPL. Results of the fitting

procedure on several sets of soil moisture retention and hydraulic conductivity data with the different optimization object functions show that, although the MDPL requires more computational efforts, it does show the best fit.

Nowadays, several soil physical databases are available, both with raw and clustered data. Data clustering usually takes place by categorizing soil samples into certain soil textural classes to determine averaged soil physical functions for such soil classes. In Chapter 3 it was shown that the classification system used in preparing the Staring Series doesn't necessarily lead to different hydrological behavior between the distinguished soil units. Computations with all individual samples within a single category show large deviations between samples with respect to computed plant evaporation ratios, soil evaporation and seepage/percolation data. So, use of averaged soil physical functions may lead to significant different outputs.

Regarding the simulation of transient 1-dimensional soil moisture flow, the software package SoWaM (Soil Water Management) was developed, as discussed in Chapter 4. SoWaM consists of a MySQL database and a number of executables. The database, called SoWaMData, is the heart of the system. Every executable reads data from it or stores data in it. The most important executable is SoWaMCalc. It solves the Richards' equation for one-dimensional moisture flow by means of the Finite Element Method. Boundary conditions may be stored in the database on an arbitrary time basis. Soil physical properties may be characterized by either the Mualem-Van Genuchten equations or by cubical splines. Four different irrigation criteria are included in the model: i) the ratio of actual and potential plant evaporation drops below a critical value; ii) a critical pressure head at a specified depth is reached, ii) a critical moisture content at a specified depth is reached and iv) the available volume of water in the root zone is less than a specified value. Output data of the model (consisting of all terms of the water balance and the pressure head and moisture content values of each node) is stored into the database at user-defined time intervals. Other applications are SoWaMFit (fits a number of cubical splines through measured data of the soil moisture retention curve or hydraulic conductivity curve), SoWaMSoil (shows the stored soil physical relationships graphically), SoWaMDrain (yields a table representing the drainage flow in relation to the groundwater level) and SoWaMVis (presents the output of the calculation in graphical and tabular ways). Compared to other well-known models, SoWaM has some specific advantages which are further specified in Chapter 4.

Though coarse-textured soils occur at several places around the world, relatively little is known about their soil physical properties. Also, virtually no information can be found in available soil physical databases like the Staring Series or others. To gain more insight in the soil physical properties of coarse-textured soils and their hydrological behavior, the physical properties of artificially created soil mixtures with different textures were determined using Wind's evaporation method. Results are described in Chapter 5. Additionally, the effect of 10 vol. % organic matter addition upon soil moisture flow was studied. The soil moisture retention and hydraulic conductivity relationships of the different mixtures were determined and their hydrological behavior was studied using the numerical model SoWaM. As expected, both texture and organic matter addition considerably affected hydraulic properties. When used as rootzone mixtures for constructing golf greens, the related irrigation water requirements dramatically differ despite that all samples in this study fall into the official USGA-specifications for constructing golf greens.

In Chapter 6 it was investigated how irrigation application and scheduling on a golf course can be optimized using a numerical model. For a golf course in the southern part of The Netherlands irrigation records were available for the greens and these were compared with numerically computed quantities using the SoWaM model. Results indicated that computed and applied irrigation amounts were almost the same on a yearly basis, however, the days of irrigation differed. Basically, the greenkeeper irrigated insufficiently during the first phase of the growing season while later on sometimes over-irrigation took place in periods where there was no real need.

In certain studies detailed monitoring of soil water contents is on-going on small spatial scale to reveal information on 2-dimensional flow behavior in dependence of the actual weather conditions. Such measurements yield large amounts of data, and therefore visualization is a handy tool for interpreting the data. In Chapter 7, a software package is described consisting of several tools to process these large amounts of measured data and to create animated movies of the changes in soil moisture content against time. Results show that water infiltration and transport through grass-covered sandy soil is more complex than currently assumed.

Samenvatting

Hoofdstuk 1 van dit proefschrift beschrijft de problemen waarvoor getracht is een oplossing te vinden. Nauwkeurige en betrouwbare bodemfysische eigenschappen zijn van cruciaal belang bij het simuleren van niet-stationaire onverzadigde stroming van water en het transport van opgeloste stoffen. Deze gegevens worden in het algemeen verkregen door veld- en laboratoriummetingen. Uit deze metingen worden dan de parameters van de Mualem – Van Genuchten vergelijkingen bepaald. Het fitten van de vergelijkingen door de gemeten waarden leidt echter niet altijd tot goede resultaten. Een database met bodemfysische eigenschappen van Nederlandse bodems (de Staringreeks) toont een tekort aan gegevens over gronden met een grove textuur, hetgeen de toepasbaarheid vermindert. Het model SoWaM en de spline interpolatie van de bodemfysische eigenschappen worden toegepast in een case –studie op de golfbaan. Er is gebrek aan visualisatietechnieken om de grote hoeveelheden gegevens te verwerken die tegenwoordig met automatische meetsystemen worden verkregen. Oplossingen voor al deze vragen en problemen zijn samengevoegd in dit proefschrift.

Door de problemen met het fitten van de Mualem-Van Genuchten vergelijkingen door een serie gemeten waarden ontstond de behoefte aan een nieuwe en eenvoudige (wiskundige) beschrijving van de bodemfysische eigenschappen. Bij een kubieke spline-benadering wordt een functie beschreven door een aantal continue 3de graads polynomen. De parameters van deze splines worden zodanig gekozen dat de functie zelf, de eerste afgeleide en ook de tweede afgeleide continu zijn in elk punt. De wiskundige achtergrond van deze splines is beschreven in Hoofdstuk 2 van dit proefschrift. De coördinaten van de eindpunten van de splines (de zogenaamde Virtual Data Points) zijn voldoende om de hele spline-functie mee te bepalen. Om de optimale ligging van deze punten te bepalen is een eenvoudige optimalisatiemethode (Controlled Random Search) toegepast. Elke optimalisatiemethode minimaliseert of maximaliseert een doelfunctie. De meest gebruikte doelfunctie is de som van het

kwadraat van het verschil tussen gemeten en berekende waarden bij eenzelfde x-waarde. Op deze manier wordt alleen de verticale afstand van een punt tot een gefitte lijn meegenomen. De Gemiddelde Afstand tussen Punt en Lijn (engels: Mean Distance from Point to Line, MDPL) wordt hier geïntroduceerd als de gemiddelde afstand tussen een aantal punten en een lijn. In dit hoofdstuk worden 5 verschillende doelfuncties vergeleken: de som van de afwijkingen, de som van het kwadraat van de afwijkingen, de som van de relatieve afwijking tussen gemeten en berekende waarde, de som van de verhouding tussen gemeten en berekende waarde en de MDPL. Het minimum aantal Virtual Data Points benodigd voor een goede fit is geschat. Voor alle toegepaste datasets is het optimale aantal Virtual Data Points gelijk aan 7. Als meer punten worden beschouwd dan wordt alleen de benodigde rekentijd groter maar zal de optimale waarde van de doelfunctie nauwelijks lager worden. Resultaten van de optimalisaties voor meerdere datasets met gegevens van pF-curves en geleidingsvermogens worden getoond met de verschillende doelfuncties. Hoewel de MDPL meer rekentijd vraagt, levert deze doelfunctie de beste resultaten.

Tegenwoordig zijn meerdere bodemfysische databases beschikbaar met zowel ruwe als samengevoegde gegevens. Het samenvoegen van gegevens vindt gewoonlijk plaats door de bodemmonsters in te delen in een aantal textuurklassen en vervolgens de gemiddelde bodemfysische karakteristieken per textuurklasse te bepalen. In Hoofdstuk 3 is aangetoond dat dergelijke classificatiesystemen, ook gebruikt in de Staringreeks, niet noodzakelijk leiden tot verschil in hydrologisch gedrag tussen de klassen. Berekeningen met alle individuele monsters binnen een klasse tonen grote verschillen tussen de resultaten van de monsters onderling wat betreft berekende verhoudingen tussen actuele en potentiële plantverdamping, bodemverdamping en kwel/wegzijgingswaarden. Het gebruik van gemiddelde bodemfysische parameters kan dus leiden tot afwijkende uitkomsten.

Ten behoeve van het simuleren van niet-stationaire één-dimensionale grondwaterstroming is het numerieke model SoWaM (Soil Water Management) ontwikkeld. Het is beschreven in hoofdstuk 4. SoWaM bestaat uit een MySQL database en een aantal programma's. De database, SoWaMData genoemd, is het hart van het pakket. Elk programma leest zijn invoergegevens uit de database en/of schrijft zijn uitvoer ernaartoe. Het belangrijkste programma is SoWaMCalc. Dat lost de Richards vergelijking voor niet-stationaire eendimensionale grondwaterstroming in de onverzadigde en de verzadigde zone numeriek op met behulp van de Eindige Elementen Methode. Randvoorwaarden op willekeurige tijdstippen kunnen worden opgeslagen in de database. Bodemfysische eigenschappen kunnen worden beschreven door ofwel de Mualem-Van Genuchten vergelijkingen ofwel door middel van de Virtual Data Points van een reeks cubical splines. Er zijn vier mogelijke criteria voor het toedienen van een beregeningsgift: i) de verhouding tussen actuele en potentiële plantverdamping komt beneden een kritieke waarde; ii) de drukhoogte op een te specificeren diepte wordt lager dan een kritieke waarde; iii) het vochtgehalte op een te specificeren diepte wordt lager dan een kritieke waarde; iv) de hoeveelheid vocht in de wortelzone komt beneden een kritieke waarde. Uitvoergegevens (bestaande uit alle termen van de waterbalans en de drukhoogte en het vochtgehalte in alle knooppunten) worden weggeschreven naar de database met een vast (door de gebruiker te specificeren) tijdsinterval. Andere programma's zijn SoWaMFit (fit een aantal splines door de gemeten waarden van een pF- of een doorlatendheidscurve), SoWaMSoil (toont de opgeslagen bodemfysische eigenschappen grafisch), SoWaMDrain (levert een tabel met drainagefluxen afhankelijk van de grondwaterstand) en SoWaMVis (toont de resultaten van de berekeningen grafisch en als tabel).

Hoewel bodems met een grove structuur over de hele wereld voorkomen, is er weinig bekend over hun bodemfysische eigenschappen. Dit soort materiaal wordt onder andere veel gebruikt bij het aanleggen van golfbanen en andere sportvelden om er zeker van te zijn dat er een voldoende afvoercapaciteit is van overtollig regenwater om zo plasvorming te voorkomen. Aan de andere kant heeft dit materiaal een buitengewoon laag vochthoudend vermogen zodat er in droge periodes regelmatig beregend moet worden. Om meer inzicht te krijgen in de bodemfysische karakteristieken van dergelijke grof-gestructureerde materialen en hun hydrologisch gedrag, zijn er in het laboratorium kunstmatige monsters gecreëerd. Hoofdstuk 5 beschrijft de wijze waarop dit is gedaan. De bodemfysische eigenschappen zijn gemeten. Ook is het effect onderzocht van het toevoegen van 10 vol. % organische stof op de eigenschappen van de monsters. Het hydrologisch gedrag van de materialen is onderzocht met behulp van het model SoWaMCalc. Zoals verwacht hebben zowel de textuur als het organische stofgehalte een grote invloed op de bodemfysische eigenschappen. De doorlatendheid neemt significant toe met toenemende grofheid. Aan de andere kant verlaagt het toevoegen van organische stof de doorlatendheid bij verzadiging met een factor 10 tot 100 en neemt het vochthoudend vermogen aanzienlijk toe. Door het toevoegen van organische stof nam de hoeveelheid beschikbaar water toe met 144% bij de enigszins grove materialen en met 434% bij de erg grove materialen. De United States Greenkeepers Association (USGA) heeft een aanbeveling uitgebracht voor de granulaire samenstelling van de toplaag van de bodem van een golfbaan. Deze aanbeveling geeft op elementaire wijze aan welke gronden geschikt zijn voor de opbouw van greens en welke korrelgrootteverdeling kan worden gebruikt voor dit doel. Er worden geen relaties met beregeningsbehoeftes gegeven. Modelsimulaties tonen aan dat de hoeveelheid beregening die nodig is om het gras in optimale conditie te houden, sterk verschilt tussen de mengsels, ondanks het feit dat zij allemaal voldoen aan de USGA aanbevelingen.

In Hoofdstuk 6 is onderzocht hoe de beregening van een golfbaan kan worden geoptimaliseerd door gebruik te maken van een numeriek model. Op een van de golfbanen in het zuiden van Nederland had een ervaren greenkeeper de beregeningsgiften bijgehouden die hij op de greens had gegeven. De gemeten vochtgehaltes op 5 cm diepte zijn gebruikt om het irrigatiecriterium te calibreren. Daarna zijn voor een andere periode de irrigatiegiften van de greenkeeper vergeleken met die zoals geadviseerd door het numerieke model SoWaMCalc. Het model adviseerde praktisch hetzelfde aantal beregeningsgiften als de greenkeeper had gegeven, maar wel op andere dagen. Het toont aan dat de toepassing van een model in samenwerking met een ervaren greenkeeper kan leiden tot een beter irrigatie management.

In bepaalde onderzoeken wordt er een gedetailleerde monitoring van vochtgehaltes in de bodem uitgevoerd om informatie te verschaffen over het twee-dimensionale gedrag van bodemvocht in relatie tot de actuele weersomstandigheden. Deze metingen leveren een enorm aantal meetwaarden op en daarom kan visualisatie helpen bij de interpretate van de gegevens. In Hoofdstuk 7 is een software pakket beschreven dat uit meerdere programma's gericht op het visualiseren van grote hoeveelheden gegevens. Er worden animatiefilmpjes gemaakt van de veranderingen van het vochtgehalte in de tijd. Resultaten tonen aan dat water infiltratie en transport in een met gras bedekte zandige bodem complexer is dan in het algemeen wordt aangenomen.

List of symbols

Symbol	Definition	Dimensions	Units
C	Differential moisture capacity	L^{-1}	cm^{-1}
d	Median particle diameter	L	mm
E_p^p	Potential plant evaporation	LT^{-1}	mm d^{-1}
E_p^a	Actual plant evaporation	LT^{-1}	mm d^{-1}
E_s^p	Potential soil evaporation	LT^{-1}	mm d^{-1}
E_s^a	Actual soil evaporation	LT^{-1}	mm d^{-1}
E_t^p	Potential evapotranspiration	LT^{-1}	mm d^{-1}
f	Mathematical function		
f	Empirical factor	-	-
g	Function		
g	Multiplication factor to obtain U_r^a from U_r^p	-	-
H	Hessian matrix		
H	Total head	L	cm
h	Pressure head	Cm	
h_a	Air entry value	L	cm
K	Hydraulic conductivity	LT^{-1}	cm d^{-1}
K_{ij}	Hydraulic conductivity for flow in direction j due to gradient in direction i	LT^{-1}	cm d^{-1}
K_s	Saturated hydraulic conductivity	LT^{-1}	cm d^{-1}
LAI	Leaf Area Index	L^2L^{-2}	m^2m^{-2}
l	Emperical parameter	-	-
MDPL	Mean distance between point and line		
m	Parameter	-	-
N	Number of data	-	-
N_d	Number of samples in class	-	-
N_p	Number of parameters	-	-
N_x	Number of state variables	-	-
N_y	number of output data	-	-
n	Measure of pore-size distribution	-	-
P	Precipitation	LT^{-1}	mm d^{-1}
p	Parameter vector		
q_b	Flux through the bottom of the considered profile	LT^{-1}	mm d^{-1}
q_d	Drainage flux	LT^{-1}	mm d^{-1}
q_{max}	Maximum steady-state flux reaching the surface	LT^{-1}	cm d^{-1}
q_u	Maximum steady-state flux reaching the surface computed with Staring class	LT^{-1}	cm d^{-1}
S	Sink term representing drainage or root extraction	T^{-1}	d^{-1}
SSQ	Sum of squares		
t	Time	T	d
U_r^p	Potential root water uptake per unit length	T^{-1}	d^{-1}
U_r^a	Actual root water uptake per unit length	T^{-1}	d^{-1}

x	Independent variable of a function	-	-
x	Vector with state variables		
x_I	Coordinate in i^{th} direction	L	cm
y	Function value	-	-
y	Measured output data		
$\hat{y}$	Output vector with estimated values		
z	Vertical coordinate	L	cm
z_g	Position of groundwaterlevel	L	m
α	Parameter related to the inverse of the air entry suction	L^{-1}	cm^{-1}
α	Parmeter for linear interpolation	-	-
β	Parameter for linear interpolation	-	-
γ	Parameter used in spline interpolation	-	-
$\gamma(y, \hat{y})$	Objective function		
$\delta((x_i,y_i),\Omega)$	Distance between point $(x_i;y_i)$ and geometrical figure Ω		
η	Parameter used in spline interpolation	-	-
θ	Volumetric moisture content	L^3L^{-3}	cm^3cm^{-3}
θ_r	Residual volumetric moisture content	L^3L^{-3}	cm^3cm^{-3}
θ_s	Volumetric moisture content at saturatio	L^3L^{-3}	cm^3cm^{-3}
ρ_j	j^{th} x-value when discretisizing function		
σ_j	j^{th} y-value when discretisizing function		
Ω	Geometrical figure in space R^2		
ω	Weight factor	-	-

Curriculum Vitae

Jan Gerrit Wesseling was born in 1953 in Wageningen. After primary school (Van de Brink school) he went to the high school (Wagenings Lyceum) where he received the diploma of HBS-B in 1971. In 1972 he started his study Land and Water Management at the Agricultural University in Wageningen with a major in mathematics and minors in Information Technology, Measuring Technique and Control Engineering, and Hydrology and Hydraulics. After his graduation in 1978 he started working at the Institute for Land and Water Management Research (Instituut voor Cultuurtechniek en Waterhuishouding) as a researcher within the section Agrohydrology of the Water Management department. He was performing research in the field of the flow of water and heat in the unsaturated zone, developed a lot of software and was involved in numerous projects. In 1998 he took the opportunity to combine his work and his hobby and became a software engineer at the Group Software Engineering of Alterra. Besides developing numerical models he dealt with designing databases, expert systems and visualization software. Since 2004 he continued his career as a hydrologist/software engineer within the Soil Physics and Land Use team of Alterra. Since that time Jan Wesseling was involved in field measurements of moisture contents and their processing and visualization, storing measured data in databases, developing new numerical models on moisture flow and irrigation requirements and evaluating the effects of surfactants on the moisture status of golf courses. These activities resulted in quite a lot of papers in scientific journals and more popular magazines, and finally to composing this thesis.

Jan Wesseling is married with Monique and they have 5 children: Piotr, Klaudia, Marian, Marcin and Patryk.

PE&RC PhD Education Certificate

With the educational activities listed below the PhD candidate has complied with the educational requirements set by the C.T. de Wit Graduate School for Production Ecology and Resource Conservation (PE&RC) which comprises of a minimum total of 32 ECTS (= 22 weeks of activities)

Review of Literature (5.6 ECTS)
- Literature review on "Soil physical data and modelling soil moisture flow"

Title of Proposal (7 ECTS)
- Flow and transport in coarse textured media (2007)

Post-Graduate Courses (5.6 ECTS)
- PHLO-Cursus "Systeemanalyse en simulatie"(in samenwerking met Groep Landbouwwiskunde); PHLO(1989/1990)
- PHLO-Cursus "Expertsystemen: ondersteuning naar menselijke maat"; PHLO (1991)
- PHLO-Cursus "Software-engineering: kwaliteitsverbetering in research & development; PHLO (1996)
- Sampling for natural resource monitoring; Alterra (2008)

Deficiency, Refresh, Brush-up Courses (14.1 ECTS)
- Diploma Fortran programmer (self study); IBM (1972)
- Diploma Basic programmer (self study); Dirksen Elektronika Arnhem (1978)
- Diploma SDK-85 soft and hardware (self study); Dirksen Elektronika Arnhem (1979)
- Certificate Assembly programmer (self study); Dirksen Elektronika Arnhem (1980)
- GENSTAT; DLO (1994)
- Delphi-4 foundation course; Oosterkamp Training and Consultancy (1998)
- DLO-In-Company training "OO-Think"; Serc, Utrecht (1998)
- DLO-In-Company training "OO-modelling"; Serc, Utrecht (1998)
- Het (om)bouwen van applicaties voor het inter/intranet; Oosterkamp Training and Consultancy (1999)
- Seminar Component-based development; Shared Objects (1999)
- Implementatie van Object-oriented ontwerpen; Serc, Utrecht (2000)
- Uncertainty and sensitivity analysis (self study); Biometris (2006)

Competence Strengthening / Skills Courses (5.6ECTS)
- Schrijven van handleidingen bij software; DLO (1992)
- Schriftelijk rapporteren; DLO (1992)
- Middle Management; Nationale Handels Academie (1993)
- Projectmatig werken; Kern Consult, Bussum (1994)

Discussion Groups / Local Seminars and Other Meetings (7 ECTS)
- Regular meetings of project teams, steering committees and advisory boards (1978-2008)
- Monthly meetings of the term Land Use and Soil Physics (2004-2008)

International Symposia, Workshops and Conferences (4.3 ECTS)
- Symposium Agrohydrology; Wageningen (1987)
- Unsaturated Flow in Hydrological Modeling; Arles, France (1988)
- Unsaturated Zone Modelling: Progress, Applications and Challenges; Wageningen (2004)
- Modelcare 2005; Scheveningen (2005)

Courses in which the PhD Candidate Has Worked as a Teacher
- International Course on Land Drainage; ILRI (1996); 1 day
- International Course on Land Drainage; ILRI (1997); 1 day
- International Course on Land Drainage; ILRI (1998); 2 days