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Uncertainty in soil physical data at river basin scale

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Abstract

For hydrological modelling studies at the river basin scale, decision makers need guidance in assessing the implications of uncertain data used by modellers as an input to modelling tools. Simulated solute transport through the unsaturated zone is associated with uncertainty due to spatial variability of soil hydraulic properties and derived hydraulic model parameters. In general for modelling studies at the river basin scale spatially available data at various scales must be aggregated to an appropriate scale. Estimating soil properties at unsampled points by means of geostatistical techniques require reliable information on the spatial structure of soil data. In this paper this information is assessed by reviewing current developments in the field of soil physical data uncertainty and adopting a classification system. Then spatial variability and structure is inspected by reviewing experimental work on determining spatial length scales for soil physical (and soil chemical) data. Available literature on spatial length scales for soil physical- and chemical properties is reviewed and their use in facilitating change of spatial support discussed. Uncertainty associated to the derivation of hydraulic properties from soil physical properties in this context is also discussed.

1 Introduction

The scope of this paper is on the issue of providing guidance on classification and quantification of uncertainty associated with soil physical- and chemical data in the unsaturated zone at the river basin scale. The underlying idea for the present paper is inspired by the need for providing guidance for the assessment of uncertain soil data targeted towards practitioners within hydrological modelling. For performing environmental hydrological modelling studies for assessing implications of politically imposed measures for the reduction of environmental pollution there is a need for decision-makers to evaluate the results of modelling studies against the background of uncertain data input needed for a comprehensive assessment of the effect of measures and

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associated costs. Questions posed by decision-makers regarding how confident they can be about simulated measures having implications for cost-effectiveness are most relevant. This has called for research relevant policy-making and integrating social and physical perspectives on environmental problems, that traverse a range of political and geographic scales (Brown and Heuvelink, 2005). Outcomes of environmental modelling studies are never certain due to uncertainty in model parameterization, boundary conditions of the model and also due to uncertainty in the model itself. The latter uncertainty arises from the fact that the hydrological model always is a more or less crude simplification of the reality in nature. Represented soil processes in the model do only capture real processes approximately. In this paper a model is defined as a numerical code that is imposed on an interpretation of the environmental system, which processes it mimics. The representation of the environmental system itself is also often called a model in literature, but in the context of the present paper the model that is representing the environmental system is denoted a conceptual model. For instance, parameterization of a groundwater model requires a correctly interpreted geological model. In this case the groundwater model is the numerical model, e.g. MODFLOW, and the interpreted geological model is the conceptual model (Refsgaard et al., 2006). Focus here is thus on making transparent to user groups the uncertainty related to spatial soil physical data at the river basin scale required for the parameterization of a model for environmental hydrological studies.

2 Soil physical and chemical properties in the vadose zone

The soil system represented by soil physical properties is a very complex system and result from physical, chemical and biological processes over time. The soil has been recognized as a key compartment in biochemical cycles (carbon, nitrogen, water, etc.) and underlying physico-chemical processes are still only partly understood and subject of research (Gratwohl et al., 2004). The variation of the soil system is in fact so complex that no description of it can be complete and so prediction is inevitably uncertain

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(Heuvelink and Webster, 2001). Soil properties can vary over time as a result of impact by climate and land management. However, in this paper only spatial variation is considered over the time scale relevant for environmental assessments within e.g. the EU Water Framework Directive (WFD), i.e. a few decades. One of the major causes for uncertainty and erroneous understanding of causal relationships and the magnitude of parameters and trends has been identified as the scale problem. Different levels of heterogeneity are encountered when passing from the microscopic to the macroscopic scale. Processes identified and regarded valid at one scale may not hold at another spatial scale. At the field scale, the modelling of nitrate leaching may focus on the influence of natural variation in the soil, but at the larger farm scale the variation in land-use will be much more important (Heuvelink and Pebesma, 1999). This scaling issue remains one of the largest problems in soil science and hydrology and various techniques have been developed to scale soil physical properties (refer to Pachepsky et al. (2003) for a comprehensive review). In soil physics, the description of water flow in soils is based on gradients in soil water potential, which in soils is predominantly determined by capillary and gravitational forces. This concept has been applied and thoroughly tested at the scale of a soil column. Predictions of water flow at larger scales are therefore an extrapolation based on the assumption that the hydraulic properties of the soil, determined at the local scale, may represent the properties at a larger scale.

In this paper soil physical data is closely linked to soil hydraulic properties, like retention data and hydraulic conductivity. Soil hydraulic properties can be derived from basic soil physical properties like texture from general purpose soil maps using pedo-transfer functions (PTFs; Bouma, 1989; Børgesen and Schaap, 2005; Rawls et al., 1991; Wösten, 1997; Pachepsky et al., 1996, 2006) and are needed for parameterization of hydrological models used to describe water- and solute transport through the vadose zone. Soil hydraulic properties may also be measured directly from samples in the laboratory and the soil hydraulic conductivity may be determined in-situ in the field (e.g. Mohanty et al., 1994; Severino et al., 2003), but this procedure is often cumbersome and expensive and therefore not feasible in practice at the scale of the river

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basin. The water flow direction in the vadose zone is often assumed to be vertical only. Vogel and Rath (2002) provide a review of flow and transport in the unsaturated domain at various spatial and temporal scales and also covering modelling aspects. The groundwater zone is the saturated domain and water- and solute transport may be represented in 3-D. Therefore, model simulated flow is dependent on knowledge of the geological structure to ensure a realistic conceptual model of the system at hand. Uncertainty related to parameterization of groundwater models is dealt with elsewhere (Nilsson et al., 2006¹).

Environmental risk assessment in which an evaluation of the uncertainty associated with pollutant fate modelling for decision making within a hydrological context are currently receiving a vast amount of interest (see e.g. Dubus and Brown (2003) for a review on uncertainty associated with pesticide fate modelling, and e.g. Worrall et al. (2002) and Søvik et al. (2003) for a review on uncertainty in a more general geochemical context. Quinn (2004) argues that the modeller must use the appropriate type of model at the appropriate scale for modelling of nitrate leaching in order to best understand nitrate losses at that scale and appreciate associated uncertainty. One of the primary contributors to the uncertainty in contaminant concentration predictions is uncertainty in the hydraulic parameters of soils at a site (e.g. Meyer et al., 1999), but geochemical properties, like CEC and pH, also play an important role (Grathwohl et al., 2003, 2004). Sensitivity analyses with the Danish DAISY model (Hansen et al., 1991) showed that nitrate variations in soil texture substantially affects nitrate leaching (Watertech, 2005). The amount of organic matter in the soil affects both hydraulic properties and mineralization. Organic pollutants (e.g. pesticides) are characterised by compound specific properties such as sorption and degradation and heavily dependent on both the soil physical and the soil chemical environment. Refer to Wauchope et al. (2002) for a review on pesticide soil sorption parameters, Delle Site (2000) for a review on factors affecting sorption of organic compounds in water systems for selected pollutants, and

¹Nilsson, B., Højbjerg, A. L., Refsgaard, J. C., and Trolborg, L.: Uncertainty in geological and hydrogeological data, *Hydrol. Earth Syst. Sci. Discuss.*, in review, 2006.

Beulke et al. (2000) for a review on simulation of pesticides on the basis of laboratory data. Geochemical and biological processes are predominant factors of the fate and transport of contaminants in soils and the unsaturated zone. Often these processes are studied separately. Detailed modelling approaches have been developed to couple the description of water flow and geochemical interactions as well as microbiological processes. They are functionally strongly related, where small-scale heterogeneity serves as an important factor to provide a niche for surviving organisms (Grathwohl et al., 2004). Leaching of contaminants through the soil is controlled by many environmental parameters and their effect on contaminant release is to a very large extent compound specific. E.g., leaching of heavy metals is heavily dependent on pH, presence of dissolved organic carbon and changes in redox potential (van der Sloot et al., 2004). Heavy metals and other toxic elements are thus subject to a complex speciation in the unsaturated zone. The conceptual approach of interface interaction between solid compounds (including complex minerals and natural organic matter) is well developed, but the validation of the different concepts and the quantification of related parameters is still uncertain and subject to scientific discussion (Grathwohl et al., 2004). Volatile compounds (VOCs) leach to groundwater unless biodegraded by microorganisms which in turn depend on other geochemical conditions for their existence. Other compounds such as various complex organic mixtures are also biodegradable, but may be very persistent over many decades to centuries. The same applies to some types of pesticides. Further environmental and compound specific parameters that influence on biodegradation include biodegradability, bio-availability and concentration of the contaminant, soil temperature, oxygen content, water content and nutrients content. Thus within the context of the Water Framework Directive and ecological status, the uncertainties associated to geochemical environmental characterisation important to potential leaching of contaminant is large and highly pollutant specific. Numerical modelling of organic pollutant leaching to groundwater is only possible if i) a detailed characterisation of the soil hydraulic and geohydrologic conditions are known, i.e. water content profile, water table elevation and hydraulic conductivity; ii) a good estimate of

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location, quantity and composition of contaminant is available and iii) good estimates of biodegradation rates for each contaminant are available. Søvik and Aagaard (2003) found that most geochemical parameters are distributed normally or lognormally. Typical values and parameter bound cannot be provided due to their site-specific nature.

5 More specific parameters that relate to geochemical conditions substantially add to the overall uncertainty. Overall guidelines with respect to uncertainty in contaminant transport are supplied in the GRACOS report (Grathwohl et al., 2003).

The uncertainty associated with the sorption parameter K_d can be placed into three major categories (Meyer et al., 2004): i) Experimental uncertainty (errors due to measurements), ii) Sorption process chemistry uncertainty (variation in solution chemistry, i.e. complexation, competitive adsorption and alteration of the adsorption-site chemistry; variation in surface adsorption sites, i.e. mineralogy and surface coatings/fracture fillings), and iii) uncertainty resulting from changing the spatial support from laboratory to field. Wauchope et al. (2002) derived information on the uncertainty in sorption in the form of 'rules of thumb'. The authors considered that i) the batch experiment probably varies from the true average K_d in the field of the same soil by a factor of two; ii) the variability in K_d in the field is to be attributed to variation of the organic matter content in the field and of the organic matter itself and typically has a CV of approximately 50%; (3) a K_d determined for different soils will vary by approximately one order of magnitude; (4) a CV of 30–60% is common in multi-soil studies and reflects the variability in the sorption capacity of the organic matter and in the measurement of the organic carbon content; and (5) Sorption (K_{oc}) values reported for different studies with multiple soils are expected to vary by an order of magnitude. The application of a similar approach for other key model input parameters would be useful. A number of sensitivity analyses have demonstrated that predictions of pesticide fate models for leaching will mainly be influenced by sorption and degradation parameters (Boesten, 1991; Soutter and Musy, 1998; Dubus et al., 2003) and hydrological parameters (Dubus and Brown, 2002; Wolt et al., 2002).

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3 Spatial- and temporal variability

Uncertainty in soil physical and geochemical data at the river basin scale will arise from the spatial and temporal variability of environmental variables, from sampling procedures in the field, and from analysis in the laboratory. Soil variability is the product of soil-forming factors operating and interacting over a range of spatial and temporal scales. Heuvelink and Webster (2001) provide a thorough review of spatial and temporal variability and used techniques to analyse them. Soil properties vary in time, but usually so slowly that it can be ignored at time scales common for hydrological studies. Agricultural management practices can significantly affect the structure of the soil and thereby structure dependent soil hydraulic properties such as preferential flow in space and time (e.g. Green et al., 2003). Frost and thaw cycles may also alter soil structure and thereby the soil physical properties (Hinman and Bisal, 1968; Moore, 1981). Recognition of the importance of spatial variability on land-use has led to the study of soil heterogeneity. In agriculture, information about the spatial structure of soil chemical and physical properties is needed to evaluate potential crop yield. In environmental science, knowledge of soil variability is needed for practical applications such as hydrologic modelling work. For example, selection of a suitable remediation method with regard to a contaminated site, as well as its implementation, requires knowledge of the heterogeneity of the properties affecting transport and degradation of pollutants. Previous work on soil heterogeneity related to environmental issues have often focused on the saturated hydraulic conductivity as this property is assumed to be one of the most important transport related properties (Søvik et al., 2003). Mulla and McBratney (2000) compiled values for the coefficient of variation for selected soil properties using data from Jury (1986), Jury et al. (1987), Beven et al. (1993) and Wollenhaupt et al. (1997) classified according to typical CV ranges (Wilding, 1985). A summary of their findings is shown in Table 1.

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4 Characterisation of uncertainty in environmental data

A general framework for assessing and representing uncertainties in environmental data is provided by Brown (2004). In this framework, a coding of attribute uncertainty categories is proposed in which a measurement scale can be:

- continuous numerical, e.g. monthly precipitation data
- discrete numerical, e.g. number of rain gauges in a catchment
- categorical, e.g. soil type

All of these measurement scales may or may not vary in space and/or time.

A distinction is made how uncertainty can be described, i.e. whether this can be done by means of i) probability distributions or upper and lower bound, ii) some qualitative indication of uncertainty, or iii) some indication of how a variable may vary. Further, the “methodological quality” of an uncertain variable can be assessed by expert judgement, e.g. whether or not instruments used are reliable and to what degree, or whether or not experiment for measuring an uncertain variable where properly conducted. Finally, the “longevity” of uncertain information can be evaluated, i.e. to what extend does the information on the uncertainty of a variable change over time.

In the following, selected variables from Table 1 are classified according to their uncertainty category, type of empirical uncertainty, methodological quality and longevity as well as data support, i.e. typical sample size (Table 2). In Table 3 the classification of uncertainty is provided for various derived hydraulic properties as well as the data support. In Tables 2, 3 and 4 the uncertainty category for all variables and parameters except one are judged to be C1, i.e. continuous numerical and varying in space, not in time. The methodological quality for all parameters is classified as “I3”, “S3” and “O4” as instruments used are well suited for field experiments, sample design adequate and approved standard in well established discipline. Longevity is judged to be “L2” as the associated uncertainty does not change within the WFD timeframe. However, close to

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the soil surface properties may change significantly due to agricultural practice. This is not accounted for here as properties are considered to be of inherent character. At depths deeper than the A- and perhaps B-horizon geochemical properties are more stable over time.

5 Spatial support for soil physical properties

Handling spatial heterogeneity, the existence of preferred time and space scales for soil processes, and approaches to finding linkages between scales of state variables, parameters and conceptualizations have been topics for research for quite a while and a review of recent ideas in this field is well beyond the scope of this paper. Blöschl and Sivapalan (1995) provide a thorough review of scale issues in hydrological modeling and Pachepsky et al. (2003) on scaling methods in soil physics. Modelling of soil processes at the scale of the river basin involves the use of measured soil data at different scales and upscale information to the scale of the applied model. Heuvelink and Pebesma (1999) distinguish between aggregation and disaggregation versus up-scaling and downscaling, where the latter is related to modeling. In this context it is convenient to refer to the 'support' being defined as the integration volume or aggregation level and often in literature a synonym to "scale". The notion of support is important to characterize and relate different scales in soil physics. Any research of soil physical properties is made with specific support and spatial spacing, the latter being distance between sampling locations. If properties are to be used with different support, e.g. when model inputs require a different support than the support of the observations, scaling becomes necessary (Heuvelink and Pebesma, 1999; Zhu and Mohanty, 2003). Soil samples taken in the field for determination of soil physical properties are typically in the order of magnitude of 100 cm^3 . For clayey soils larger samples would be more appropriate in order to capture preferential pathways (e.g. Kay and Angers, 2003). Simulation models are support dependent (e.g. Heuvelink and Pebesma, 1999) and field data sampled for model input is often at a support much

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smaller than the support of interest for model output. Therefore it is needed to aggregate to move from point support to, say, field support. First aggregating point support to field support and then running a hydrological model, or by first running the model using point support data and then aggregating the model results may do this. Usually, the models used are non-linear and the two alternatives for aggregation will not yield the same result (e.g. Addiscot, 1993; Heuvelink, 1998). Deriving parameters for closed-form soil water retention expressions like the Gardner-Russo (Gardner, 1958; Russo, 1988), the Brooks and Corey (Brooks and Corey, 1964), Campbell (Campbell, 1974) or van Genuchten model (van Genuchten, 1980) may be done by means of PTFs based on i) a spatial classification of soil texture by general purpose soil maps or by ii) spatial interpolation of soil data. Advantages and disadvantages of both methods are discussed in Heuvelink and Webster (2001). Variability within soil mapping units is also described in Mulla and McBratney (2000) where they identify two types of variation of soil physical properties: i) soil variability within soil mapping units, and ii) variability caused by mapping and classification error. For most of the soil mapping in the US the scale allows up to 40% of the region within a soil mapping unit to consist of dissimilar inclusions.

A large number of articles have reported on the spatial variability of pesticide residues or leaching in the field as mentioned in the review paper by Dubus et al. (2003). Also a number of leaching-risk studies have attempted to account for soil variability within map units to predict leaching of nitrate (Gorres and Gold, 1996; Richter et al., 1998; Webb and Lilburne, 2005). The above-mentioned works have been attributed to some extent to the variability in space of soil physical and geochemical properties, which in turn influence predictions of both nitrate and pesticide leaching models. Causes of spatial variability are traditionally classified into intrinsic or extrinsic factors. Taking the agricultural soil system as an example, intrinsic variability is the variability caused by natural conditions in soil whereas extrinsic variability is that imposed on a field as part of land management practices. Examples of soil characteristics that exhibit intrinsic variations are texture and mineralogy while tillage, fertilizer

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and pesticide applications, harvesting and removal of crop residues all contribute to the development of an extrinsic variability.

6 Geostatistics for representing spatial variation

Often, soil properties do not occur across the landscape in a random fashion. Soil physical properties taken at close spacings will be similar or spatially correlated whereas samples from distant samples may be dissimilar and spatially uncorrelated. The spatial correlation structure of soil physical- and chemical properties can be used to estimate properties at unsampled locations by means of geostatistics (Journel and Huijbregts, 1978; Hamlett et al., 1986; Isaaks and Srivastava, 1989; Cressie, 1991). An introduction to geostatistics applied to soil science is provided by e.g. Heuvelink and Webster (2001) and a textbook by Nielsen and Wendroth (2003). Only the very essential theory needed for understanding the principle of autocorrelation is repeated below. Input for distributed hydrological modeling at the river basin scale typically requires that available sampled data at point support is aggregated to block support data that is compatible with the model grid scale. For soil physical properties this usually involves modeling the spatial correlation structure using the semi-variogram $\gamma(h)$ (Burgess and Webster, 1980) followed by spatial interpolation (kriging).

$$\gamma(h) = \frac{1}{2n(h)} \sum_{i=1}^{(n)h} [z_i - z_{i+h}]^2 \quad (1)$$

where h is the separation distance between the measured soil properties z_i and z_{i+h} at locations x_i and x_{i+h} . The number of pairs separated at distance h is denoted $n(h)$. In Eq. (1) it is implicitly assumed that $\gamma(h)$ is only dependent on h and not on the positions x_i and x_{i+h} . At very small separation distances, observations should become very similar and the semivariogram, i.e. the variance of (z_i, z_{i+h}) theoretically approaches zero. In practice there will often be an intercept (the nugget) that accounts

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for the uncorrelated component of the variance as well as random measurement errors. At larger distances h , the semivariance typically flattens out and becomes constant, i.e. observations become uncorrelated. The distance h where this occurs is called the range. The semivariogram can also be expressed by the autocorrelation function, which is related to the semivariogram by:

$$\gamma(h) = s^2 [1 - \rho(h)] \quad (2)$$

Where s^2 is the process variance and $\rho(h)$ is the autocorrelation function. The semivariogram can be modelled by fitting experimental sampling data to a model. The most common models in this respect are the linear, spherical and exponential. If experimental data is not available then one must rely on values for typical autocorrelation lengths from the literature in order to do spatial interpolation (kriging). Describing uncertainty using geostatistics is not an activity exempt from uncertainty itself as variogram uncertainty may be large (Jansen, 1998) and spatial interpolation may be undertaken using different techniques.

7 Experimental autocorrelation length scales for soil physical properties

In this section an overview of experimentally determined autocorrelation length scales is provided and summarized in Tables 5, 6 and 7. Russo and Bresler (1981) reported length scales for several hydraulic properties: 21 m for saturated hydraulic conductivity (K_{sat}), 55 m for saturated water content, 25 m for residual water content and 35 m for sorptivity. Later Vauclin et al. (1983) found correlation length values around 25 m for water content at pF 2.5. Cook et al. (1989) found a range of 120 m for the recharge rate of groundwater in Australia as related to saturated conductivity. A joint research project in Denmark (Jensen and Refsgaard, 1989) investigated and described the nature of the spatial variability of some soil physical properties on the basis of detailed experimental studies on two different localities, a clayey and sandy site, and at different depths by means of geostatistical methods. They found no textural spatial dependence for the

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clayey site nor for porosity, dry bulk density and K_{sat} , whereas the available water content showed spatial dependence for all depths. At the sandy site, no spatial dependence was found for silt, humus, dry bulk density, porosity and soil water characteristics at 10 kPa. For clay, correlation lengths of 20 m have been reported and for fine sand and coarse sand approximately 45 m. Mohanty et al. (1994) conducted a spatial analysis of measured hydraulic conductivity using disc infiltrometers and found no spatial dependence for K_{sat} and the van Genuchten retention parameter. Kristensen et al. (1995) studied two fields in Denmark representing sandy loam and a sandy clay loam within the context of site specific farming. They derived correlation lengths for a number of soil physical and chemical parameters. Romano and Santini (1997) analysed within the Basilicata area in Southern Italy semivariogram models for curve fitted (RETC; van Genuchten et al., 1991) and estimated retention characteristics using a PTF approach (Gupta and Larson, 1979; Rawls et al., 1982; Rawls and Brakensiek, 1989; Vereecken, 1989). They arrived at spherical semi-variogram models and ranges between 800 and 1300 m for both fitted and PTF estimated water retention data. Neuman and Wierenga (2003) used omnidirectional sample variograms and fitted spherical models for percent sand, silt and clay at depths 0–30 cm. Similar variograms for underlying 30–180 cm can be found in Wang (2002). Some appeared to fit a linear or Gaussian model, but most fitted spherical models with ranges of 20–25 m. They also conducted a variogram analysis of the hydraulic parameters K_{sat} and saturated water content (θ_s) obtained by neural network software package ROSETTA (Schaap et al., 2001). Most of them fitted spherical models with ranges between 20 and 36 m. Recently Sobieraj et al. (2004) studied scale dependency in spatial patterns of saturated conductivity in a tropical rainforest catena and a list of previous studies on the spatial structure of K_{sat} and correlation lengths varying from 1–25 m. Leij et al. (2004) found that topographic attributes can be used to improve the prediction of soil hydraulic properties using PTFs and neural network techniques. Within the context of spatial structure of soil physical structure and agriculture Delcourt et al. (1996) studied the spatial structure of soil nutrients from two fields in the main agricultural area in Belgium and reported geostatistical parameters

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for some topsoil nutrients. Later McBratney and Pringle (1999) conducted a literature review on variograms for soil- and soil chemical properties for use in precision agriculture. In their study they presented an overview of variograms for pH, clay- and sand content, carbon-, NO₃-N-, phosphorus- and potassium content in the soil. Mulla and McBratney (2003) compiled various sources of experimental work on semivariogram models for several measured soil and agronomic properties from Jury (1986), Warrick et al. (1986), Wollenhaupt et al. (1997) and McBratney and Pringle (1997). These results and others are summarized in Tables 5–7. Geostatistical analyses have also been performed to study the spatial variability of pesticide sorption (e.g. Jacques et al., 1999) and degradation (e.g. Walker et al., 2001) in the field. Also soil nitrate has been geostatistical analysed with respect to the content in the topsoil (e.g. Huang et al., 2004), in the soil profile (e.g. Shahandeh et al., 2004), or in the whole vadose zone (e.g. Onsoy et al., 2004).

8 Uncertainty related to derivation of soil hydraulic properties for hydrological model input

Water retention and hydraulic conductivity are crucial input parameters in any modelling study on water flow and solute transport in soils. Uncertainty involved in deriving soil hydraulic properties from pedotransfer techniques is discussed in this section. In Table 6 examples of parameters are listed which are of large importance for hydrologic studies with focus on parameterization of modelling tools for describing water- and contaminant flow through the unsaturated zone towards the groundwater zone. All hydraulic properties and thus derived model parameters relate to soil composition and are highly uncertain at the river basin scale as soil texture data is usually extracted from regional databases and is based on measurements from soil profiles that may be located a quite long apart. Derivation of soil hydraulic properties for input to modelling tools either by i) soil class PTFs, e.g. Carsel and Parrish (1988) and Wösten (1995), ii) linear/non-linear regression equations (regression PTFs), e.g. Rawls and Braken-

siek (1985) or Minasny et al. (1999) iii) curve fitting, e.g. RETC (van Genuchten et al., 1991) or finally iv) through the neural network approach, e.g. ROSETTA (Schaap et al., 2001) are all associated with substantial uncertainty. PTFs transfer experimentally collected data, usually texture properties (but also variables like organic matter or pH), to parameters required by numerical models. In most cases such parameters are related to hydraulic properties, but PTF may also predict soil chemical characteristics, e.g. CEC, soil phosphorus and adsorption-desorption parameters (Wösten et al., 2001) as well as mechanical and biological properties (McBratney et al., 2002). As opposed to the categorical (USDA soil classes) soil physical parameter estimation, PTFs usually are continuous functions for providing such estimates. Wösten et al. (2001) reviews PTFs based on the European HYPRES (Wösten et al., 1999) and the international UNSODA (Leij et al., 1996; Nemes et al., 2001) databases. PTFs may require a fixed dataset, e.g. textural properties or be hierarchical depending on the available data input (Schaap et al., 1998, 2001). McBratney et al. (2002) developed a decision support system in which PTFs are automatically selected to ensure a minimum variance and return soil physical and chemical properties with their uncertainties based on the information provided. They also provide a comprehensive review of PTFs and related uncertainty. This uncertainty can be due to the uncertainty of the PTF model itself and to uncertainty in the input data. The uncertainty associated with the model can be calculated from the non-parametric bootstrap method (Efron and Tibshirani, 1993). The uncertainty of the input data can be computed using Monte Carlo simulation. This is done by sampling repeatedly from the assumed distribution of the input data and evaluation of the output of the PTF model. Finke et al. (1996) concluded from a study in the Netherlands that uncertainty in PTFs required adequately capturing the variability of basic soil properties as well as water table depths if leaching of chemicals is studied. Wösten et al. (2001) evaluated accuracy and reliability of PTFs in general and discussed statistical techniques in this respect. Typical examples for PTF accuracy (RMSE) for water retention data were also presented. RMSE of volumetric water content at pressure heads of -33 kPa and -1500 kPa ranged for each of those

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tensions from 0.02 (Pachepsky et al., 1996) to $0.11 \text{ m}^3 \text{ m}^{-3}$ (Schaap et al., 1998). Wösten et al. (2001) concluded that in general PTFs can be considered to be sufficient accurate and reliable and may be appropriate for many applications on regional and national scale. If PTFs are trained/calibrated adequately, the uncertainty in the model is usually smaller than the uncertainty in the inputs. One may use Latin Hypercube Sampling to sample the multivariate joint distribution of the prediction. This is achieved by sampling repeatedly from the assumed probability distribution of the input variables and evaluating the result of the PTF for each sample. The distribution of the results, along with the mean, standard deviation and other statistical measures can then be estimated (Christiaens et al., 2001; McBratney et al., 2002) compared different methods to determine soil hydraulic properties including PTF estimations through USDA soil texture classes, continuous PTFs and neural networks in combination with bootstrapping. Moreover, they analysed how this uncertainty is propagated in the distributed hydrological MIKE SHE model using a Latin Hypercube approach. Uncertainties of soil physical parameters in the range from 3 to 700% were found, K_{sat} and θ_r being the most uncertain. Neural networks performed best in terms of the total error. Schaap et al. (1998) and Schaap and Leij (1998) present a neural network analysis for hierarchical prediction of soil hydraulic properties. They used 12 neural network models for prediction of soil water retention properties and K_{sat} and demonstrated that neural network models compared favourably to regression models when tested against independent data. The hierarchical approach has the practical advantage that they permit high flexibility with respect to data input. Uncertainty in predicted soil hydraulic properties can be assessed by combining the neural network approach with the bootstrap method and is incorporated in the ROSETTA software (Schaap et al., 2001). Carsel and Parrish (1988) presented joint probability distributions for the parameters of the van Genuchten (1980) water retention and unsaturated hydraulic conductivity models (Mualem, 1976). These parameters are: saturated volumetric water content, residual volumetric water content, K_{sat} , van Genuchten model parameters α and n . Carsel and Parrish based their analysis on data from soil samples collected by the Natural Resources Conserva-

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tion Service representing soils from 42 states in USA. Soil measurements used were bulk density, percent sand (0.05–2 mm), and percent clay (<0.002 mm). Bulk density was used to infer saturated water content while percent sand and clay, along with saturated water content, were used with the regressions of Rawls and Brakensiek (1985) to estimate the remaining parameters. Carsel and Parrish's soil database included 15 737 samples from twelve USDA soil textural classifications. Meyer et al. (1997) resampled the distributions and derived closed-form distributions of the soil hydraulic parameters that can be used to represent parameter uncertainty when the information about a soil is limited to its textural class (Meyer et al., 1997). Meyer et al. (2001) listed derived dry bulk density, compiled by Meyer and Gee (1999) from the US Natural Resources Conservation Service Soil Database (NRCSSC) divided according to the USDA soil textural class. For each textural class, the Kolmogorov-Smirnov D-statistic was calculated using hypothetical normal and lognormal distributions. It appeared that a normal distribution fitted the bulk density data best for all textural classes and is therefore recommended. As described previously, for each of the NRCSSC database soil classes, the statistics for the parameters θ_s , θ_r , α , n , and K_{sat} are computed using a multiple regression equation (Carsel and Parrish, 1988). The Brooks and Corey parameters ψ_c and λ as well as the Campbell b parameter are derived from the first mentioned. Thus for each soil class, the probability density function, the mean, standard deviation (std), lower limit (ll) and upper limit (ul) is provided. Meyer et al. (1997) induced correlations between parameters by applying the correlations between θ_s , θ_r , α , n , and K_{sat} given in Carsel and Parrish (1988). The rank correlation method of Iman and Conover (1982) as employed in the Latin Hypercube sampling code of Iman and Shortencarier (1984) is used. These tables originally presented in Meyer et al. (1997) are well suited for use in generation of Monte Carlo datasets where information on the probability density function as well as mean and variance are required.

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9 Summary and conclusions

For hydrological modelling studies at the river basin scale there is a clear need to identify, classify, and quantify uncertainties associated to soil physical and soil chemical data in order to guide decision makers in assessing simulations of measures and their implications for policy making. So far very little guidance has been provided on how to cope with uncertainty in data for input to simulation models and uncertainty in the models themselves. In this paper uncertainty is restricted to field data, more specifically soil physical data. A quantification of data uncertainty for soil physical data is of crucial importance for the assessment of the reliability of simulated solute transport through the unsaturated zone to vulnerable groundwater resources at multiple scales. Environmental studies for hydrologic modelling are typically at the river basin scale and therefore there is a need to know how to handle change of support for data collected at one (usually at a far lesser) scale and the relevant river basin scale. In general for modelling studies, non-linear soil water models can only be used at the support for which they were developed. Estimating soil properties at unsampled points by means of geostatistical techniques require reliable information on the spatial structure of soil data. In this paper this information is assessed by reviewing current developments in the field of soil physical data uncertainty and adopting a classification system. Then spatial variability and structure is inspected by reviewing experimental work on determining spatial length scales for soil physical (and soil chemical) data. Quantified length scales enable change of support, e.g. by geostatistically transforming point support data to larger scales relevant for hydrologic modelling studies. Finally, the derivation of hydraulic parameters from soil physical data by means of e.g. PTFs is considered and uncertainties in this process reviewed.

It can be concluded that considering uncertainty in soil physical data in environmental hydrologic studies at the river basin scale is not as yet widely practised. Decision-makers who use the results of hydrologic modelling studies to assess the effects of various measures need guidance from modellers on how uncertainty is propagated in

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simulations and what the implications are for policymaking.

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Table 1. CV and magnitude of variability for selected properties (adapted from Mulla and McBratney, 2000).

Soil property	CV (%)	Magnitude of variability
pH	2–15	Low
Porosity	7–11	Low
Bulk density	3–26	Low to moderate
% sand	3–37	Low to moderate
0.01 MPa water content	4–20	Low to moderate
Pesticide adsorption coeff.	12–31	Moderate
Soil Organic Matter (SOM)	21–41	Moderate to high
1.5 MPa water content	14–45	Moderate to high
% clay	16–53	Moderate to high
Soil Nitrate N	28–58	Moderate to high
Soil water infiltration rate	23–97	Moderate to high
Soil available potassium (K)	39–157	High
Soil available phosphorus (P)	39–157	High
Soil electrical conductivity	91–263	High
Saturated hydraulic conductivity	48–352	High
Solute dispersion coeff.	79–178	High
Solute dispersivity	78–539	High

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Table 2. Classification of uncertainty in texture related properties. For explanation of used codes please refer to the text.

Name	Abbrev.	Uncertainty Category	Type of empirical uncertainty	Methodological quality	Longevity	Data support (sample size)
Bulk density	RHO	C1	M1	I3, S3, O4	L2	100 cm ³
Organic matter content	SOM	D1	M1	I3, S3, O4	L2	100 cm ³
Porosity	POR	C1	M1	I3, S3, O4	L2	100 cm ³

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Table 3. Classification of uncertainty in derived hydraulic properties. For explanation of used codes please refer to the text.

Name	Abb.	Uncertainty category	Type of empirical uncertainty	Methodological quality	Longevity	Data support (sample size)
Saturated water content	θ_s	C1	M1	I3, S3, O4	L2	100 cm ³
Residual water content	θ_r	C1	M1	I3, S3, O4	L2	100 cm ³
vG fitting parameter	α	C1	M1	I3, S3, O4	L2	100 cm ³
vG fitting parameter	n	C1	M1	I3, S3, O4	L2	100 cm ³
B&C air entry pressure	ψ_c	C1	M1	I3, S3, O4	L2	100 cm ³
B&C pore size distr. index	λ	C1	M1	I3, S3, O4	L2	100 cm ³
Campb. fitting parameter	b	C1	M1	I3, S3, O4	L2	100 cm ³
Saturated conductivity	K_{sat}	C1	M1	I3, S3, O4	L2	100–10 000 cm ³

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Table 4. Classification of uncertainty in geochemical properties. For explanation of used codes please refer to the text.

Name	Abbrev.	Uncertainty category	Type of empirical uncertainty	Methodological quality	Longevity	Data support (sample size)
Total phosphorus	TOTP	C1	M1	I3,S3,O4	L2	100 cm ³
Ferro oxides	FE-O	C1	M1	I3,S3,O4	L2	100 cm ³
Aluminium oxides	AL-O	C1	M1	I3,S3,O4	L2	100 cm ³
Phosphorus ferro oxides	FE-P	C1	M1	I3,S3,O4	L2	100 cm ³
Phosphorus alu oxides	AL-P	C1	M1	I3,S3,O4	L2	100 cm ³
CEC	CEC	C1	M1	I3,S3,O4	L2	100 cm ³
CaCO ₃	CaCO ₃	C1	M1	I3,S3,O4	L2	100 cm ³
PH	pH	C1	M1	I3,S3,O4	L2	100 cm ³

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Table 5. Autocorrelation length scales (ranges) for soil physical properties.

Name	Symbol	$\gamma(h)$ model	range (m) ^a	reference
Clay content	% Clay	Stepwise linear ¹ , spherical ² Exp. ³	15–40 ¹ , 20–33 ² 69 ³	¹ Jensen and Refsgaard (1989), ² Neuman and Wierenga (2003), ³ McBratney and Pringle (1999)
Silt content	% Silt	Spherical ²	N/A ¹ , 20–26 ²	¹ Jensen and Refsgaard (1989), ² Neuman and Wierenga (2003)
Sand content	% Sand	Stepwise linear ² , spherical ³ Exp. ⁴	1–34 ¹ , 15–40 ² , 20–35 ³ , 75 ⁴	¹ Mulla and McBratney (2000), ² Jensen and Refsgaard (1989), ³ Neuman and Wierenga (2003), ⁴ McBratney and Pringle (1999)
Bulk density	RHO, ρ	none ¹ , exp ²	N/A ¹ , 37–39 ²	¹ Jensen and Refsgaard (1989), ² Kristensen et al. (1995)
Organic matter content	SOM	exp. ² , spherical ⁹	34–45 ² , 112–250 ⁹	² Kristensen et al. (1995), ⁹ Mulla and McBratney (2000)
Porosity	POR	none ¹ , spherical ⁴	N/A ¹ , 55 ^{3a} , 14–76 ^{9a}	¹ Jensen and Refsgaard (1989), ³ Russo and Bresler (1981), ⁹ Mulla and McBratney (2000)
Soil water characteristics ^{1b,2c}	SWC	Stepwise linear ¹ , spherical ²	25–40 ¹ , 375–1285 ²	¹ Jensen and Refsgaard (1989), ² Romano and Santini (1997)

^a: for saturated water content

^b: water content (WC) at –10, –32, –100, –316, –1000 and –15 850 kPa; AWC (WC_100 kPa – WC_ 15 850 kPa); ln(Ksat)

^c: WC at –1, –10 and –100 kPa

Table 6. Autocorrelation length scales (ranges) for derived soil hydraulic properties.

Name	Symbol	$\gamma(h)$ model	range (m)*	reference
Saturated water content	θ_s	Spherical ^{1,4}	800–900 ^{1a} , 55 ^{2b} , 14–76 ³ , 20–36 ⁴	¹ Romano and Santini (1997), ² Russo and Bresler (1981), ³ Mulla and McBratney (2000), ⁴ Neuman and Wierenga (2003)
Residual water content	θ_r	Spherical ^{1c}	25 ^{1c,2} , 10–50 ^{3d}	¹ Vauclin et al. (1983), ² Russo and Bresler (1981), ³ Jensen and Refsgaard (1989)
vG fitting parameter	α	N/A ¹ , spherical ^{2c}	N/A ¹ , 25 ^{2c}	¹ Mohanty et al. (1994), ² Vauclin et al. (1983)
vG fitting parameter	n	Spherical ^{1c}	25 ^{1c}	¹ Vauclin et al. (1983)
B&C air entry pressure	ψ_c	spherical ^{1c}	25 ^{1c}	¹ Vauclin et al. (1983)
B&C pore size distr. index	λ	N/A ^{1e} , spherical ^{2c}	N/A ^{1e} , 25 ^{2c}	¹ Mohanty et al. (1994), ² Vauclin et al. (1983)
Campb. fitting parameter	b	Spherical ^{1c,2f}	25 ^{1c}	¹ Vauclin et al. (1983), ² Meyer et al. (1997)
Saturated conductivity	K_{sat}	Spherical ^{1g}	21 ^{2,3} , 120 ^{1g} , N/A ⁴ 25–40 ⁵ , 1–34 ⁶ , 20–36 ⁷ , 1–25 ⁸	¹ Cook et al. (1989), ² Russo and Bresler (1981), ³ Vauclin et al. (1983), ⁴ Mohanty et al. (1994), ⁵ Jensen and Refsgaard (1989), ⁶ Mulla and McBratney (2000), ⁷ Neuman and Wierenga (2003), ⁸ Sobieraj et al. (2004)

^a: water content at –1 kPa

^b: for saturated water content

^c: water content at pF2.5

^d: in general for retention parameters

^e: through $n=\lambda+1$

^f: relation between b and ψ_c and λ

^g: groundwater recharge rate

*: in horizontal direction

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Table 7. Autocorrelation length scales (ranges) for geochemical properties.

Name	Abbrev.	$\gamma(h)$ model	range (m)*	reference
Soil Nitrate-N	NO ₃ -N	spherical/ exp ^{2,3}	40–275 ¹ 31–120 ² 52 ³	¹ Mulla and McBratney (2000) ² Shahandeh et al. (2005) ³ McBratney and Pringle (1999)
Carbon	C	Spherical ¹	50 ¹	¹ McBratney and Pringle (1999)
Soil available potassium	K	Spherical ²	75–428 ¹ 11.4 ²	¹ Mulla and McBratney (2000) ² McBratney and Pringle (1999)
Total phosphorus	TOTP	linear/exp. ² , gaussian ^{1,2} , spherical ⁵	63 ¹ , 150–500 ² , 55 ³ , 68–260 ⁹ , 19.3 ⁵	¹ Delcourt et al. (1996), ² Kristensen et al. (1995), ³ Klironomos et al. (1999), ⁴ Mulla and McBratney (2000) ⁵ McBratney and Pringle (1999)
Ferro oxides	FE-O	Exp ¹	1.7	¹ Søvik and Aagaard (2003)
Aluminium oxides	AL-O	Exp ¹	0.48 ¹	¹ Søvik and Aagaard (2003)
Phosphorus ferro oxides	FE-P	N/A ¹	N/A ¹	¹ Søvik and Aagaard (2003)
Phosphorus alu oxides	AL-P	N/A ¹	N/A ¹	¹ Søvik and Aagaard (2003)
CEC	CEC	Exp ¹	7.5 ¹	¹ Barbizzi et al. (2004)
Soil pH	pH	Exp ²	20–260 ¹ 62 ²	¹ Mulla and McBratney (2000) ² McBratney and Pringle (1999)
CaCO ₃	CaCO ₃	linear/exp ¹	30 ¹	¹ Kristensen et al. (1995)

*: in horizontal direction