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Data assimilation of in situ soil moisture measurements in hydrological models

- First annual doctoral progress report, work plan and achievements -

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List of abbreviations

θ_s	saturated water content
A	is the tortuosity index
a	tube shape factor
CAS	central absolute sensitivity here defined
Ce	Nash–Sutcliffe coefficient of model efficiency
CPRS	central parameter relative sensitivity
CPRS	central parameter relative sensitivity
CTRS	central total sensitivity analysis
ECa	apparent soil electrical conductivity
ECw	soil water (fully saturated soil or soil solution)
EMI	electromagnetic induction
ET	evapotranspiration
ETo	reference evapotranspiration
FF	formation factor
K(h)	unsaturated hydraulic conductivity
K-C	Kozeny and Carman
Ks	saturated hydraulic conductivity
KsAm	Arithmetic mean of saturated hydraulic conductivity
KsGM	geometric mean of saturated hydraulic conductivity
L	tortuosity exponent
m	cementation exponent of
MVG	van Genuchten-Mualem
N	the depolarization factor
p	saturation index
p_f	perturbation factor
PTF	pedotransfer functions
R^2	coefficient of determination R –square
RMSE	root-mean-square deviation
S	degree of saturation
S(t)	sensitivity function
SA	sensitivity analysis
Sp	specific surface area and
TDR	time domain reflectometry
x	parameter
x_j	parameter value
y(t)	output variable
Δx_j	perturbation,
θ(h)	soil water retention curve
ρ_b	bulk density
Ψ	matric potential
ε	porosity

Management summary

Water scarcity and the presence of water of good quality is a serious public concern since it determines the availability of water to society. Water scarcity especially in arid climates and due to extreme droughts related to climate change drive water use technologies such as irrigation to become more efficient and sustainable. Plant root water and nutrient uptake is one of the most important processes in subsurface unsaturated flow and transport modeling, as root uptake controls actual plant evapotranspiration, water recharge and nutrient leaching to the groundwater, and exerts a major influence on predictions of global climate models. To improve irrigation strategies, water flow needs to be accurately described using advanced monitoring and modeling. Our study focuses on the assimilation of hydrological data in hydrological models that predict water flow and solute (pollutants and salts) transport and water redistribution in agricultural soils under irrigation. Field plots of a potato farmer in a sandy region in Belgium were instrumented to continuously monitor soil moisture and water potential before, during and after irrigation in dry summer periods. The aim is to optimize the irrigation process by assimilating online sensor field data into process based models.
Over the past year, we demonstrated the calibration and optimization of the Hydrus 1D model for an irrigated grassland on sandy soil. Direct and inverse calibration and optimization for both heterogeneous and homogeneous conceptualizations was applied. Results show that Hydrus 1D closely simulated soil water content at five depths as compared to water content measurements from soil moisture probes, by stepwise calibration and local sensivity analysis and optimization the Ks, n and α value in the calibration and optimization analysis. The errors of the model, expressed by deviations between observed and modeled soil water content were, however, different for each individual depth. The smallest differences between the observed value and soil-water content were attained when using an automated inverse optimization method. The choice of the initial parameter value can be optimized using a stepwise approach. Our results show that statistical evaluation coefficients (R^2, Ce and RMSE) are suitable benchmarks to evaluate the performance of the model in reproducing the data. The degree of water stress simulated with Hydrus 1D suggested to increase irrigation at least one time, i.e. at the beginning of the simulation period and further distribute the amount of irrigation during the growing season, instead of using a huge amount of irrigation later in the season.
In the next year, we will further look for to the best method (using soft data and methods for instance PTFs, EMI, Penetrometer) to derive and predict the spatial variability of soil hydraulic properties (saturated hydraulic conductivity) of the soil and link to crop yield at the field scale. Linear and non-linear pedotransfer functions (PTFs) have been assessed to predict penetrometer resistance of soils from their water status (matric potential, ψ and degree of saturation, S) and bulk density, ρ_b, and some other soil properties such as sand content, Ks etc. The geophysical EMI (electromagnetic induction) technique provides a versatile and robust field instrument for determining apparent soil electrical conductivity (ECa). ECa, a quick and reliable measurement, is one of ancillary properties (secondary information) of soil, can improve the spatial and temporal estimation of soil characteristics e.g., salinity, water content, texture, prosity and bulk density at different scales and depths. According to previous literature on penetrometer measurements, we determined the effective stress and used some models to find the relationships between soil properties, especially Ks, and penetrometer resistance as one of the prediction methods for Ks. The initial results obtained in the first yearshowed that a new data set would be necessary to validate the results of this part.

In the third year, quasi 3D-modelling of water flow at the field scale will be conducted. In this modeling set -up, the field will be modeled as a collection of 1D-columns representing the different field conditions (combination of soil properties, groundwater depth, root zone depth). The measured soil properties are extrapolated over the entire field by linking them to the available spatially distributed data (such as the EMI-images). The data set of predicted Ks and other soil properties for the whole field constructed in the previous steps will be used for parameterising the model. Sensitivity analysis 'SA' is essential to the model optimization or parametrization process. To avoid overparameterization, the use of global sensitivity analysis (SA) will be investigated. In order to include multiple objectives (irrigation management parameters, costs, …) in the parameter optimization strategy, multi-objective techniques such as AMALGAM have been introduced. We will investigate multi-objective strategies in the irrigation optimization.

Keywords: soil, Hydrus, modeling, water flow and solute transport, tensiometers, water content profile probes, sensitivity analysis, Ks, PTFs, ECa, model calibration, validation and optimization

Chapter 1 Introduction

1.1 Scientific background

Plants are dependent on soil water for their growth and in many cases irrigation is needed during the growing season to accommodate for this need. The efficient use of water, e.g. in irrigation, for food production is of utmost importance. Two important aspects which affect irrigation efficiency are the type of irrigation and irrigation scheduling. Optimizing the design of irrigation systems can maximize plant yield and decrease the volume of applied water. Approaching an optimum water supply for productivity (soil moisture being maintained near to the upper available water content or field capacity) is the goal of irrigation scheduling (Jones, 2004). Generally, four different approaches are used in irrigation management: i) controlling soil-water content in the root zone by its direct or indirect measurement in soil, i.e., "soil-based", ii) using meteorological data and mathematical models that calculate evapotranspiration (ET), i.e., "weather-based", iii) sensing of the plant response to water deficits by measuring crop parameters such as stem diameter, leaf thickness or stem sap flow, root pattern , i.e., "crop-based" , and iv) canopy temperature-based via infrared thermometers on land or boarded on aircrafts and/or satellites, i.e., remote sensing (Jones, 2004; Evett et al., 2008; Pardossi et al., 2009). In this study, the potential of using a a mix of these methods is explored.

In the case of soil-based irrigation scheduling, optimizing the water use needs the accurate prediction of soil-water content and soil-water potential in the root zone in order to simulate infiltration, redistribution and evaporation processes. This in turn requires the determination of hydraulic properties (Hopmans et al., 2002) and conditions related to climatology at the upper boundary and groundwater dynamics at the lower boundary of the soil profile (Gandolfi et al., 2006). Water flow and redistribution in soils is governed by hydraulic properties that can be measured in the laboratory and in the field. Soil hydraulic properties derived from direct laboratory experiments on small soil samples (e.g., ring or column samples) are often not representative for the key hydrological processes at larger spatial scales observed in the field (e.g., Ritter et al., 2003; Vereecken et al., 2008). The discrepancy between the field and laboratory determination of soil water retention characteristics, i.e., the relationship between soil water content and water potential θ(h) and the relationship between hydraulic conductivity and water potential K(h) could be attributed to the inadequate representation of large pores in the laboratory, sample disturbance and spatial variability, hysteresis and/or overburden pressure, and scale effects related to the sample size (Field et al., 1985; Shuh et al., 1988). Next to the scale issue, soil hydraulic properties are also subject to temporal changes (Alletto and Coquet 2009; Or et al. 2000), which are attributed to the changes in soil structure induced by tillage, drying-wetting cycles, solution composition, biological activities, soil erosion and settlement, compaction, shrinking and swelling due to freeze-thaw cycles (Leij et al., 2002; Suwardji and Eberbach, 1998; Genereux et al., 2008; Petersen et al., 2008; Alakukku, 1996).

It is well recognized that direct measurement of hydraulic properties -hard data- (in the field or on the laboratory) is often time consuming, labor intensive, costly, and changes or destructively samples the system. Finding a link between soft and hard data in the field could be a solution to this. Using PTFs to link hydraulic properties to other measurements such as "ECa" or penetrometer data could be a way forward to estimate the spatial ditribution of hydraulic conductivity over the whole field.

Real-time monitoring of surface and subsurface water flow flux, soil moisture, and water potential is critical if soil hydraulic properties, and their tempo-spatial variability are to be accurately determined for dynamic modeling and irrigation process optimization. Recent developments in soil sensor technology (Evett et al., 2008; Pardossi et al., 2009) allow for easy monitoring of soil moisture and water potential and these can be used to determine field soil hydraulic properties and their temporal variability.

To assess the soil water status in the root zone, evapotranspiration (ET) and precipitation are two important boundary conditions that need to be accurately assessed at the upper boundary of the soil profile (Brutsaert, 2005; Li et al., 2012 ; Nosetto et al., 2012). There are a number of studies that have examined to estimate and evaluate evapotranspiration using remote sensing (Winsemiuse et al., 2008; Lazzara and Rana, 2010) and hydrological modelling (Li et al., 2012; Nosetto et al., 2012). Root uptake of water and nutrients is considered an important process controlling water flow (recharge) and nutrient transport (leaching) to the groundwater in numerical models simulating water content and fluxes in the subsurface and thus also exerting a major influence on predictions of climate change impacts (Feddes and Raats, 2004). The common approach for estimating root water uptake through hydrological modeling is to relate the root length and mass distribution of roots to water uptake patterns.

Numerical methods are increasingly established and adopted (calibrated, evaluated and validated) for application to water resources planning and management using hydrological models. They can be applied to solve realistic field and laboratory situation problems as opposed to analytical models (Šimůnek and van Genuchten, 2008). The Hydrus-1D model (Šimůnek et al., 2008a) that is used in this study has been used in a wide range of applications in research and irrigation management (e.g., Hanson et al., 2008; Forkutsa et al., 2009; Roberts et al., 2008, 2009), water harvesting (Verbist et al., 2009), and also to simulate the fate of nutrients by evaluating and comparing fertilization strategies for different crops and contaminants in soils (e.g., Seuntjens et al., 2001, 2002a,b; Cote et al., 2003; Gärdenäs et al., 2005; Ajdary et al., 2007; Crevoisier et al., 2008).

Šimůnek and Hopmans (2002) defined calibration as the process of adjusting a model by manipulating the input parameters such as soil hydraulic parameters, initial and boundary conditions within a reasonable range, so that simulated variables match observed variables as close as possible by using for instance observed water content or pressure head data. Some methods of model calibration include trial and error, the sequential method, and automated minimization and parameter estimation techniques (parameterzation).

Soil hydraulic parameters are the most effective input parameters to derive transient water flow throught the soil. Some times measured soil hydraulic parameters should be optimized. Estimating field soil hydraulic parameters (single or multi-objective) can be done by inverse modeling (soft data) of high frequency field soil moisture and soil water potential measurements (Vrugt et al., 2008). Care should be taken when using inverse modeling whith in-situ observations collected at different scales (Dane, 1999; Musters, 2000; Scott et al., 2000; Ritter et al., 2003; Wollschläger et al., 2009). Therefore, a sensitivity analysis 'SA' (local or global) is an essential step in the model optimization process. An example of the latter is the Levenberg–Marquardt optimization (local method) for single-objective inverse parameter estimation (Abbasi et al., 2003a, b; Simunek et al., 1999; Jacques et al., 2012). Recently, multi-objective techniques such as AMALGAM have been introduced (Vrugt and Robinson, 2007) Excellent overview examples of the inverse modeling procedure can be found in Hopmans et al. (2002), Vrugt et al. (2008) and Wöhling and Vrugt (2011).

1.2 Aim of the research and research strategy

The objective of the PhD is to develop and test data assimilation methods for optimizing irrigation efficiency using a combination of sensors and process based soil hydrological models. Sensors that will be used are soil moisture sensors and online tensiometers that measure water content and water potential in a fully automated field setup for quantitatively identifying flow processes in an agriculture soil. The monitoring data are continuously used to improve the model predictions of water status in the plant root zone and therefore the steering of the irrigation.

New approaches in data assimilation will be used to improve the models. Data assimilation techniques in hydrology are thus far mostly related to integration of satellite-derived soil moisture at large spatial scales and not for local applications and in situ measurements (van Dijk and Renzullo, 2011). We will develop and test data-assimilation methods for irrigation management purposes, which are extremely relevant for arid and semi arid conditions, such as Iran, but also for the management of intensively used agricultural fields in West- and Southern Europe suffering from summer droughts related to climate change.

The specific objectives are:
1) Simulation of root water uptake in vadose zone and status of water in rhizosphere (including concentrations of solutes and nutrients or pollutants) using the Hydrus-1D model in combination with other state of the art crop based models like AquaCrop
2) Determine soil hydraulic properties based on soft data and transfer methods
3) Investigate the tempo-spatial variability of soil hydraulic properties,
4) The improvement of irrigation management using sensors and models for water flow and redistribution in soils.
5) Assimilate data from soil moisture sensors and tensiometers in hydrological models that predict water flow (and solute transport) in soils

1.3 Summary of the research of the past year

The study site is a sandy agricultural area at the border between Belgium and the Netherlands, where potatoes are grown. During the study period 2011-2012, the farmer cultivated grass. The area is flat and runoff is not considered to be important. The site was equipped with two weather stations located on the field. Soil-water content and pressure head have been recorded at several depths in the vadose zone. At each location, one tensiometer was installed horizontally at a depth of 30 cm, whereas one soil water content profile probe was placed vertically allowing to measure soil-water content at 10, 20, 30, 40 and 50 cm depths (root zone). The tensiometers, water content profile probes and weather stations were connected to a CR800 data logger. All measurements were taken on an hourly basis.
Soil samples were taken at eight locations and two depths (25 and 75 cm) to determine Ks, soil water retention curve data and some other basic soil properties. Parameters describing the soil hydraulic properties were fitted to the observed data set using RETC program for windows, version 6.02. In the topsoil layer, the organic carbon content, the silt and clay content, and total porosity and geometric Ks was higher as compared to the subsoil layer. Bulk density, sand content, arithmethic Ks and the water retention shape factors on the other hand show the opposite trend.
Simulation of water flow and grass root water uptake in the vadose zone of the field was carried out by using HYDRUS- 1D version 4.16 for 122 days in 2011. The contribution of each input parameter and factor to the uncertainty of the outputs of a model is determined by manual calibration and sensivity analysis. A stepwise calibration approach was used to evaluate the effect of soil hydraulic parameters, soil layering, and root water uptake. To assess the effect of soil hydraulic parameters on water content simulations, simulations with varying

values for Ks, n and α were conducted. The effect of soil layering was evaluated by choosing either a homogeneous or a heterogeneous profile and changing the depth of each material. Regarding root water uptake, three different root density distributions (uniform, linear decrease, and linear increase-decrease) were analysed. Results indicated that a linear decreasing root density distribution and a 45-cm-deep first layer offered the best simulation results and this was used for the initial simulations in this study. In the stepwise calibration approach the model was not sensitive to changes in soil hydraulic parameters i.e. n and α while Ks was sensitive.

To reduce the number of parameters of optimization and finalize the calibration process, local sensitivity analyses were conducted by calculating the central parameter relative sensitivity "CPRS". According to the results α, n and Ks are most sensitive (in decreasing order) and the sensitivity changed over time with the seasonal changes in water status in both soil layers.

In a third step of the modeling approach, an inverse modeling technique was applied. Determining optimal parameter values by minimizing the residuals between measured and simulated variable data is the most common approach in parameter optimization methods. In the inverse modeling process, first we optimized only the values for Ks of the two layers, taking initial values for Ks for each layer equal to the values estimated in the previous step of stepwise process, while keeping the other hydraulic parameters fixed to the measured values, and taking the thickness of the first layer equal to 45 cm and a linear root density decrease with depth. Afterward based on the SA result Ks, n and α were optimized for both layers. The root-mean-square deviation (RMSE), the coefficient of determination (R^2), and the Nash–Sutcliffe coefficient of model efficiency (Ce), were used to evaluate the difference between the observed and modeled data. It was concluded that in the automated calibration the performance criteria R^2 and Ce were higher and RMSE was lower than in the manual calibration, indicating better model performance. The 2012 data set was used for validation of the calibrated model.

Estimations of the field-scale saturated hydraulic conductivity were made using pedotransfer functions. Linear and non-linear Pedotransfer functions (PTFs) have been assessed to predict penetrometer resistance of soils from their water status (matric potential, ψ and degree of saturation, S) bulk density, ρb, and some other soil properties such as sand content, Ks etc. The final goal of the analysis is to estimate Ks from other datasets available with a higher spatial resolution using PTFs. Apparent electrical conductivity (ECa), one of the ancillary properties (secondary information) of soil, could improve the spatial and temporal estimation of some soil properties at different scales and depths. Field ECa are derived from EMI sensors which are versatile and robust field instrument for determining bulk soil electrical conductivity. An ECa dataset is available for the field site and as part of this study, the estimation of saturated hydraulic conductivity from the ECa dataset based on the empirical relations of Archie's law and Kozeny and Carman, "K-C" was assessed. Two hypothesis for this purpose were conducted. So far no hypothesis could be rejected and we need new data to validate and finalize the results.

Chapter 2 Report of the past period

2.1 Achieved Results

2.1.1 Description of study site and soil

The study site is a sandy agricultural area at the border between Belgium and the Netherlands (N 51°19'08'', E05°10'38'') where potatoes were grown. The potato farmer applies several precision agricultural practices. For irrigation, he is using sprinkler irrigation to improve potato growth in the sandy soils during dry periods in summer. During the study period 2011-2012, the farmer cultivated grass. The area is flat and runoff is not considered to be important. The fluctuation of ground water table was between 80 and 140 cm below the ground surface. The site was equipped with two weather stations (type CM10, Campbell Scientific Inc., Utah, USA) located on the field. Soil-water content and pressure head was recorded (from 4 May until 2 September 2011 in the wet zone and from 1 January 2011 until 2 September 2011 in the dry zone) at several depths in the vadose zone at two locations, A and B, in a wet and dry zone of the field respectively (Fig. 1). At each location, one tensiometer (type T4e, UMS, Munich, Germany, accuracy ±0.5 kPa) was installed horizontally at a depth of 30 cm, whereas one soil water content profile probe (type EasyAG50, Sentek Technologies Ltd., Stepney, Australia) was placed vertically allowing to measure soil-water content at 10, 20, 30, 40 and 50 cm depths (root zone). The tensiometers, water content profile probes and weather stations were connected to a CR800 data logger (Campbell Scientific Inc., Utah, USA). All measurements were taken on an hourly basis. The data set from the dry location (B) was used for the initial modeling.

Soil samples were taken to determine soil saturated hydraulic conductivity and water retention curve (undisturbed 100 cm^3 soil samples) and some soil properties such as texture, organic matter, $CaCO_3$ (disturbed soil) at two depths (0-50 cm and 50-100 cm) at eight locations along a transect (Fig. 1). The transect was chosen to account for the maximum variation in soil properties based on a geophysical survey with an EM38 proximal sensor (Geonics Ltd, Ontario, Canada) which revealed a distinct zone with increased electrical conductivity crossing the transect.

The soil water retention curve, $\theta(h)$, was determined using the sandbox method (Eijkelkamp Agrisearch Equipment, Giesbeek, the Netherlands) up to a matric head of -100 cm and the pressure plate apparatus for matric heads equal or below -200 cm, following the procedure outlined in Cornelis et al. (2005). Soil hydraulic properties were determined by fitting the parameters of the van Genuchten (vG) (van Genuchten, 1980) and Mualem model to the observed data set using the RETC program (van Genuchten et al., 1991). The saturated hydraulic conductivity (Ks) was determined using a laboratory permeameter (M1-0902e, Eijkelkamp Agrisearch Equipment, Giesbeek, the Netherlands) maintaining a constant head. The arithmetic mean of the values for each depth interval was used as an initial estimate for all scenarios and models. For Ks, besides the arithmetic mean, the geometric mean was also calculated for the calibration, since a number of field studies demonstrated that Ks is lognormally distributed rather than normally (Reynolds et al., 2000; Verbist et al., 2010). The soil properties along the transect are given in Table 1. In the topsoil layer, the organic carbon content, the silt and clay content, and total porosity and geometric mean Ks were higher as compared to the subsoil layer. Bulk density, arithmetic mean Ks on the other hand show the opposite trend. Also note that optimised saturated water content θs was lower than total porosity, as was also reported by e.g., (van Genuchten et al., 1991). This is due to a portion of the total porosity not contributing to water movement because of air entrapment and the presence of large pores draining too rapidly to become saturated and because some pores are not connected or are blocked.

Table 1. Measured physical and chemical soil properties

Soil depth	OC	CaCO3	Sand	Silt	Clay	Bulk density	KsAM	Ks GM	ε	Ɵr	Ɵs	α	n
cm	(%)	(%)	(%)	(%)	(%)	(mg m^{-3})	(cm h^{-1})	(cm h^{-1})	(m^3 m^{-3})	(m^3 m^{-3})	(m^3 m^{-3})	(cm^{-1})	
0-50	2.26	0.015	91.1	6.68	2.18	1.595	2.187	1.382	0.397	0.077	0.365	0.015	2.408
50-100	0.71	0	93.5	4.78	1.67	1.782	2.271	1.308	0.388	0.055	0.378	0.019	2.549

Ɵr, Ɵs are residual and saturate water content, respectively; α and n are shape parameters for the van Genuchten-Mualem equation, which was obtained by RETC software. Ks and ε denote the saturated hydraulic conductivity and porosity.

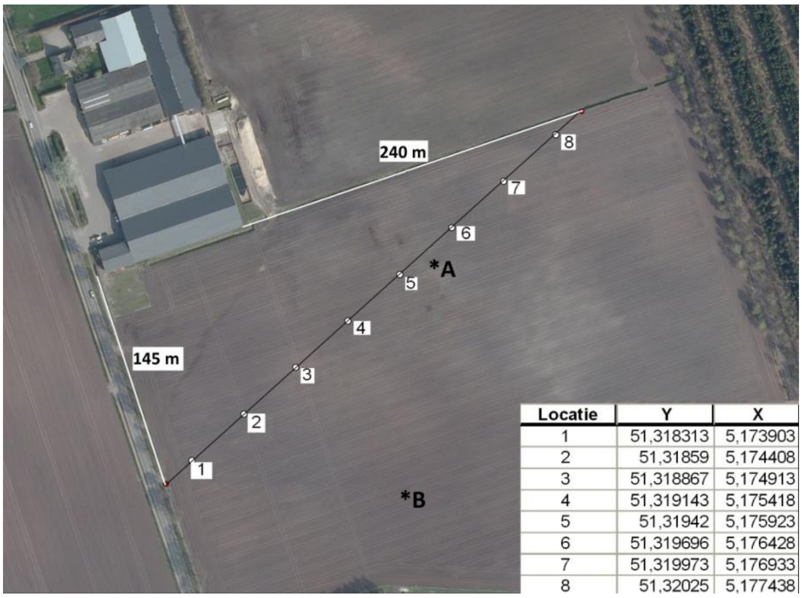


Figure 1. A map of the study site with the numbers denoting sampling points and the capital letters (A and B) representing locations of soil moisture monitoring (wet and dry zone respectively).

2.1.2: Modeling at monitoring locations

Simulation of water flow and root water uptake in the vadose zone of the field from 4 May, 2011 at 13:00 (time 1) to 2 September, 2011 at 11:00 (time 2903) was carried out by using HYDRUS- 1D version 4.16. The profile depth was 100 cm and two layers with different material properties according to the field measurements (Table 1) were chosen a priori. The van Genuchten-Mualem (MVG) soil hydraulic model without air entry value and hysteresis was used. Initial water content for the calibration periods was set to observed water contents of 0.037, 0.048, 0.048, 0.066 and 0.102 m^3 m^{-3} at a depth of 10, 20, 30, 40 and 50 cm, respectively. The boundary conditions for water flow were an atmospheric boundary condition with surface runoff for the upper and free drainage for the lower boundary condition. The pore connectivity parameter of the MVG model was fixed at l=0.5 (Schaap and Leij, 2000; Wöhling and Vrugt, 2011; Verbist et al., 2012). The Feddes model (Feddes et al., 1977) without solute stress was used for root water uptake. Default values for grass (Taylor and Ashcroft, 1972) provided with Hydrus 1D were used.

2.1.2.1: Model calibration

The contribution of each input parameter and factor to the uncertainty of the outputs of a model is determined by sensitivity analysis. A stepwise calibration approach (initial calibration) was used to evaluate the effect of a) soil hydraulic parameters, b) soil layering, and c) root water uptake on water content simulations. To assess the effect of soil hydraulic parameters on water content simulations, simulations with varying values for Ks (between 0.1-20 cm h-1; with all other parameters fixed to measured values), for n (between 1-5; all other parameters fixed to measured values), and α (limited between 0.001-0.1; all other parameters fixed to measured values) were conducted.

The effect of soil layering was evaluated by changing the depth of the two soil materials (first and second layer), and by considering a homogeneous profile (one layer of soil) by calculating the effective Ks based on soil layer thickness. Regarding root water uptake, three different root density distributions (uniform, linear decrease with maximum at the soil surface and zero value at the bottom of root zone, and increase from the ground surface to depth of 50 cm followed by a decrease from 50 cm to 100 cm) were analysed. Results (not shown here) indicated that a linear decreasing root density distribution and a 45-cm-deep first layer offered the best simulation results and this was further used for the simulations in this study. The effect of soil layering was evaluated by changing the depth of the two soil materials (first and second layer), while keeping all other hydraulic parameters fixed for both layers. The 45-cm-deep first layer was the best result with measured soil Hydrualic parameter values in this step. The model was not sensitive to changes in soil hydraulic parameters α and n in the initial calibration but this was further investigated in the systematic sensitivity analysis SA. The statistical goodness-of-fit for the simulations of the initial calibration with measured hydraulic values are summarized in table 2.

Table 2. Statistic criteria for the fit between measured and simulated soil water content at different depths in initial calibration approach.

Statistic criteria	Observation nodes- Depth (cm)				
	10	20	30	40	50
R2	0.678	0.755	0.775	0.773	0.805
RMSE	13.227	11.886	4.307	2.185	6.022
Ce	-1.045	-0.816	0.514	0.648	-8.611

R2, RMSE and Ce are the coefficients of determination, the root-mean-square deviation, and the Nash–Sutclife coefficient of efficiency.

2.1.2.2: Sensitivity analysis (SA) approach

Local sensitivity analysis was conducted by linking the following equations in the Python software and Hydrus 1D. Sensitivity analysis was defined as a “sensitivity study" of the uncertainty in outputs of a mathematical model or system (numerical or otherwise) to changes in the uncertainty of parameters, inputs or initial conditions which are often poorly known. Local and global sensitivity analysis are two large categories of sensitivity analysis. Generally in model calibration purposes, the local sensitivity analysis has been used to find the most relevant parameters. Local sensitivity analysis methods have a relevance to small changes of parameters, while global methods concern the effect of simultaneous, possibly orders-of- magnitude parameter changes (Saltelli et al., 2008). To reduce the number of parameters that need to be optimized, local sensitivity analyses are often performed that evaluate model output for each parameter perturbation in a one-at-a-time approach (Verbist et al., 2012). A dynamic sensitivity function can be written as follows:

$$S(t) = \frac{\partial y(t)}{\partial x} \qquad (1)$$

Where S(t), y(t) and x denote sensitivity function, output variable and parameter respectively. If an output variable (y) significantly changes due to the small changes of an interested parameter (x), it is called sensitive to the parameter.

This partial derivative can be calculated analytically or numerically with a finite different approach by local linearity assumption of the model. Local sensitivity functions evaluate the partial derivative around the nominal parameter values. The central differences of sensitivity function are used to rank the parameter sensitivities and can be expressed as follows:

$$\Delta x = p_f . x_j \qquad (2)$$

$$CAS \; = \frac{\partial y(t)}{\partial x} = \lim_{\Delta x_j} \frac{y(t, x_j + \Delta x_j) - y(t, x_j - \Delta x_j)}{2\Delta X_j} \qquad (3)$$

$$CTRS = \frac{\partial y(t)}{\partial x} . \frac{Xj}{y} \, , \qquad CPRS = \frac{\partial y(t)}{\partial x} . xj \qquad (4)$$

where p_f is the perturbation factor, x_j is the parameter value and Δx_j is the perturbation, CAS is the central absolute sensitivity, CTRS is the central total sensitivity analysis and CPRS is central parameter relative sensitivity.

Figure 2 illustrates the results of the SA as a function of time for α, n and Ks. A perturbation factor of 0.01 could be better but smaller perturbation factors are not possible given the output accuracy of Hydrus-1D so a perturbation factor 0.1 was chosen. During SA analysis of each parameter at specific layer, the value of other parameters was fixed to the average of the measured values. According to the results α, n and Ks are sensitive in both layers and the sensitivity is largest for α, then n and finally Ks. The results also show for all parameters a change in sensitivity with time with the seasonal changes in water status.

2.1.2.3: Inverse estimation

Determining optimal parameter values by minimizing the residuals between measured and simulated variable data is the most common approach in parameter optimization methods. A period between 1304 h (27 June 20:00) and 2903 h (2 September 11:00) was chosen as the inverse simulation period for each of the five depths, which means that we had 8016 soil-water content records with hourly precipitation and evaporation input data. In this part of the study Hydrus 1D is run inversely using simulations of soil water content to optimize the values for α ,n and Ks of the two layers (based on SA). Furthermore the layer depth was also optimized. The best result was obtained for a thickness of 30 cm for the first and 70 cm for the second soil layer. The results of the parameter optimization and the performance criteria calculated for the fit between measured and simulated soil water content (water flow) for the case of the 30 and 70 cm depth of layers are presented in table 4. The best simulated time series of soil water content with the inverse modeling are depicted in figure 3. Results show the inverse model overestimates the simulated data at 30 and 40 cm depth during the first half of the simulation period. During the optimization the α and n values increased and decreased respectively. The Ks value decreased for the first layer (to 1.899 cm h^{-1}) and increased for the second layer(to 99.082 cm h^{-1}).

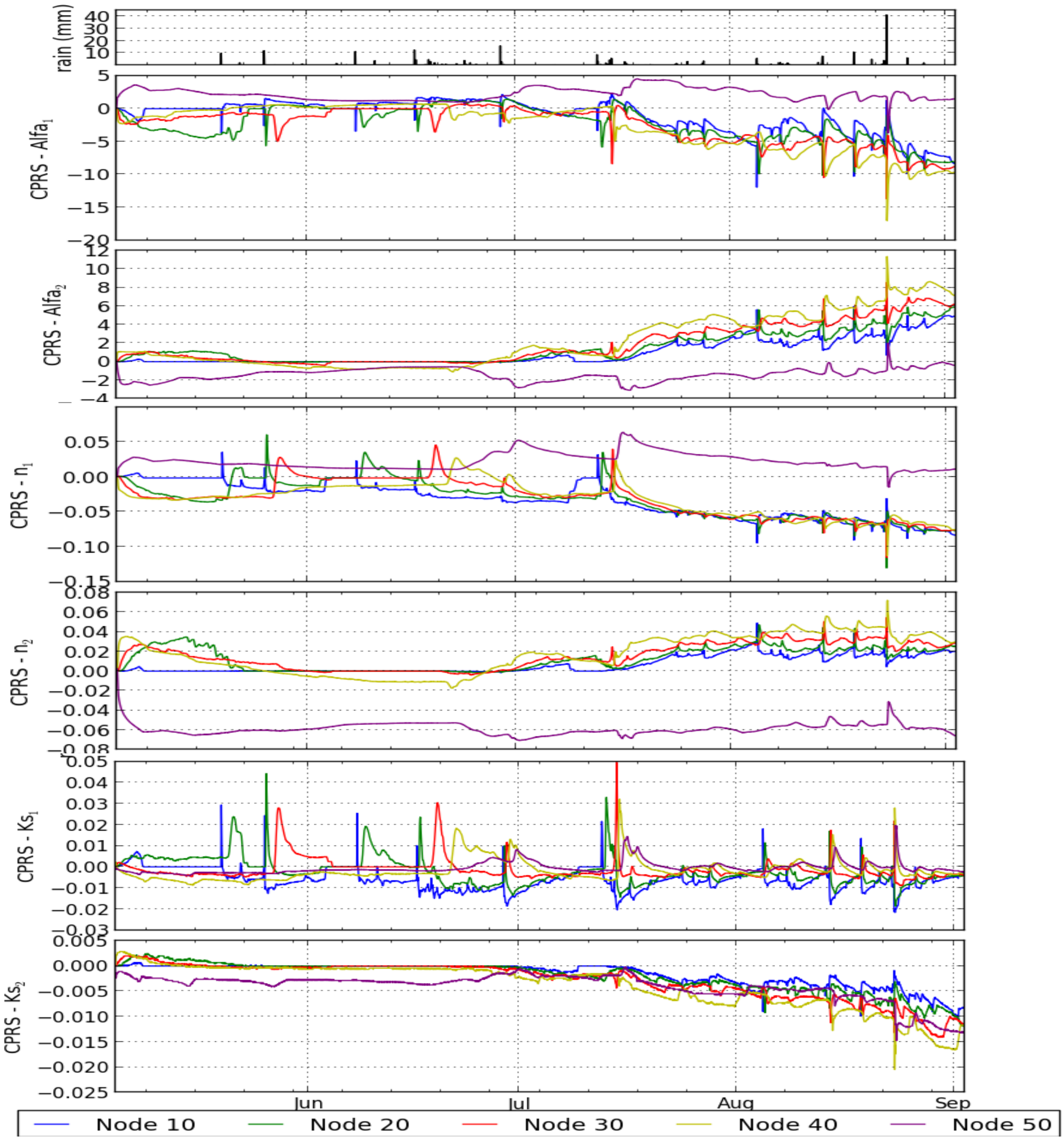


Figure 2. The sensitivity analysis "SA" results for parameters as a function of time. The number 1 and 2 correspond to first and second layer.

Table 4. Optimized hydraulic parameters for 30 and 70 cm depth of layers and calculated performance criteria for the fit between measured and simulated soil water content .

	Parameter	Optimized value	Lower	Upper	RSQ	Mass balance error
First layer	α (cm^{-1})	0.036288	00.034677	0.037899	0.841	0.243%
	N	1.2459	1.2392	1.2525		
	Ks ($cm\ h^{-1}$)	1.899	1.7226	2.0753		
Second layer	α (cm^{-1})	0.025826	0.021846	0.029806		
	N	1.3019	1.2909	1.3129		
	Ks ($cm\ h^{-1}$)	99.082	70.001	128.16		
	Depth (cm)	10	20	30	40	50
Performance criteria	R^2	0.834	0.922	0.775	0.769	0.780
	RMSE	4.107	2.743	5.365	2.420	1.087
	Ce	0.803	0.903	0.245	0.568	0.687

R^2, RMSE and Ce are the coefficient of determination, the root-mean-square deviation, and the Nash–Sutcliffe coefficient of efficiency ($cm^3 cm^{-3}$).

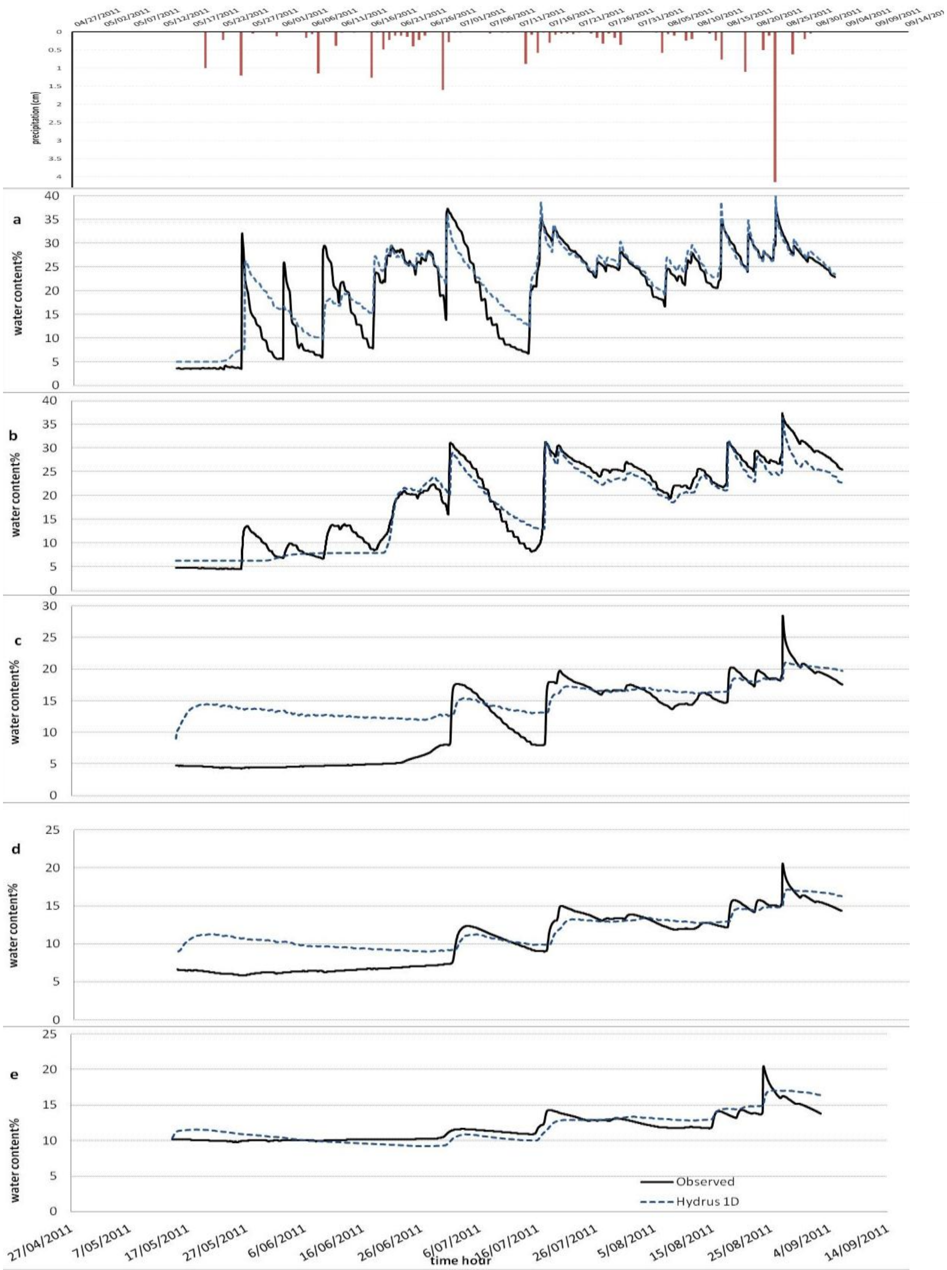


Figure 3. Observed and simulated time series of soil water content with inverse modeling for 30 and 70 cm depth of layers at a) 10, b) 20, c) 30, d) 40 and e) 50 cm depth.

2.1.2.4: Model validation

For validation purposes, the optimized values were used to simulate water flow and root water uptake in the vadose zone from 1 March, 2012 at 00:00 (time 1) to 25 November, 2012 at 23:00 (time 6480). The statistical goodness-of-fit criteria for the simulations are depicited in table 5. The best simulated time series of soil water content are shown in Figure 4.

Table 5. Statistic criteria for the fit between measured and simulated soil water content at different depths in validation approach.

Statistic criteria	Observation nodes- Depth (cm)				
	10	20	30	40	50
R^2	0.521	0.457	0.094	0.133	0.098
RMSE	4.579	4.004	6.486	3.225	5.269
Ce	0.945	0.941	0.886	0.935	0.692

R^2, RMSE and Ce are the coefficients of determination, the root-mean-square deviation, and the Nash–Sutclife coefficient of efficiency.

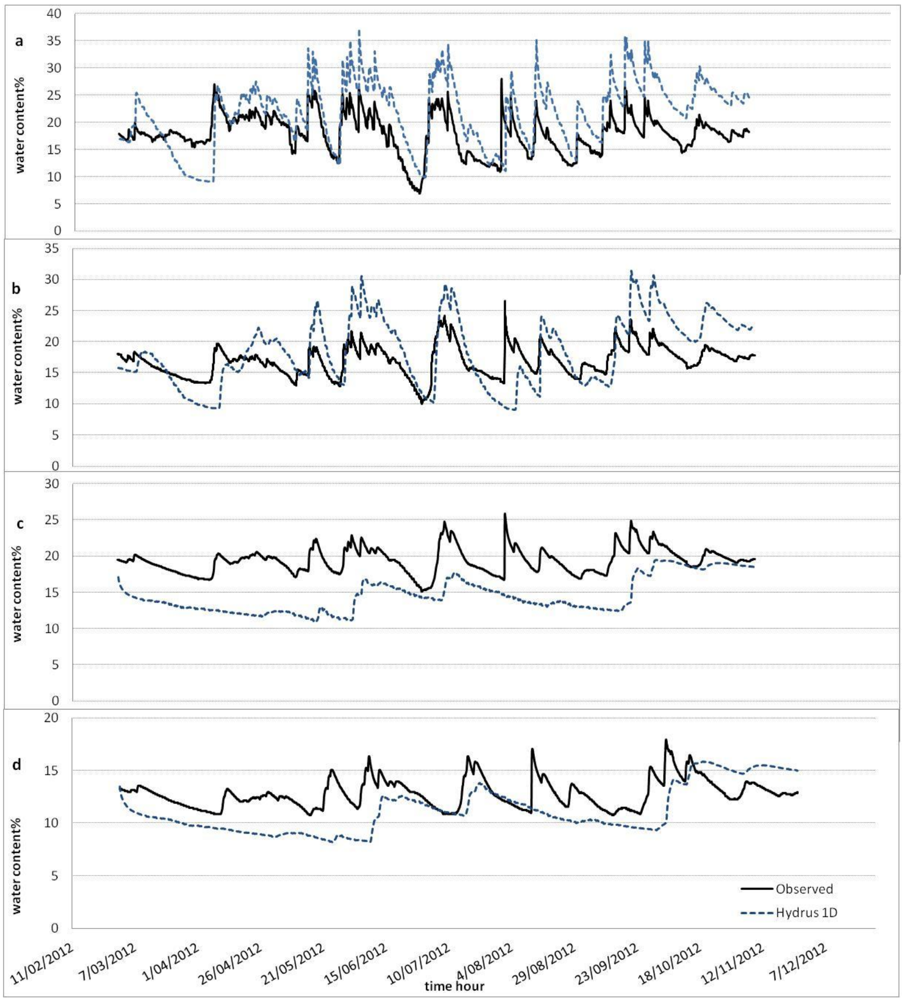


Figure 4. Observed and simulated time series of soil water content for 30 and 70 cm depth of layers at a) 10, b) 20, c) 30, and d) 40 cm depths for validation period.

2.1.3: Field scale Ks determination by Pedotransfer functions (PTFs)

2.1.3.1: Penetrometer dataset and soil physical properties

Field estimates of the saturated hydraulic conductivity were made using pedotransfer functions based on other available measurements such as penetrometer resistance and soil physical properties. Linear and non-linear pedotransfer functions (PTFs) have been tested to predict penetrometer resistance of soils from their water status (matric potential, ψ and degree of saturation, S) bulk density, ρ_b, and other soil properties such as sand content, Ks etc. The aim of this analysis is to estimate Ks from other available datasets with a higher spatial resolution using PTFs. According to literature on penetrometer measurements, we determined the effective stress and used some PTF equations to find the relationships between soil properties, and pentrometer resistance as one of the prediction ways of Ks. We concluded that the results were not satisfactory with the limited set of soil properties available and new measurements are necessary to further evaluate this.

2.1.3.2: Apparent electrical conductivity (ECa) dataset and soil physical properties

The Electromagnetic induction (EMI) technique provides a versatile and robust field instrument for determining apparent soil electrical conductivity (ECa). ECa measurements with EMI sensor, a DUALEM-21S sensor (DUALEM, Milton, ON, Canada), were already conducted to map the depth to a contrasting textural layer in the our field site. Details about the method of ECa measurements with the DUALEM-21S sensor can be found in Saey et al. (2009). ECa, a quick and reliable measurement, is one of the ancillary properties (secondary information) of soil and could improve the spatial and temporal estimation of some soil properties at different scales and depths. The interesting question for our study is “can unsaturated and saturated hydraulic conductivity (field-scale) be predicted from ECa data?”. The correlations between ECa data and hydraulic properties were investigated in order to find Ks (spatial scale) based on ECa data.

The estimation of saturated hydraulic conductivity from the ECa dataset based on the empirical relations of Archie’s law and Kozeny and Carman, “K-C” has been assessed. Empirical Archie’s law (1942) and theoretical equations of Sen et al., (1981) are used by many researchers to describe the electrical conductivity in clean sandstone, non-clean sand, gravel aquifer, sedimentary rocks and porous media (Cosentini et al., 2012;Doussan and Ruy, 2009; Friedman and Seaton, 1998;Huntley, 1986; Khalil and Santos, 2009; Morin et al., 2010; Niwas and de Lima, 2003; Sen et al., 1981; Slater, 2007). The formation factor equation can be written as:

$$FF = \frac{ECw}{ECa} \qquad (5)$$

Where ECw and ECa denote soil water (fully saturated soil or soil solution) and bulk soil electrical conductivity or apparent electrical conductivity respectively. Another formulation is:

$$FF = A\varepsilon^{-m} \qquad (6)$$

Where A is the tortuosity index ($A=(Le/L)^2$) related to the type of rock and porous media (often determined by regression methods). ε is porosity and m defined as the porosity exponent , cementation index or shape factor. In ideal conditions, normally A=1 (not tortuosity and Le=L); For high-porosity granular materials such as soils, we typically set m=1.5, and for consolidated rocks with lower porosity, we typically use a cementation exponent of m=2.0 (Sen et al., 1981; Mendelson and Cohen, 1982; Sen, 1984; Robinson and Friedman, 2001). Lesmes and Friedman (2005) mentioned the following equation for spherical grains:

$$m = \frac{5-3N}{3(1-N^2)} \qquad (7)$$

With N the depolarization factor (Jones and Friedman, 2000) defined as:

$$N(a) = \frac{1}{1+1.6(a/b)+0.4(a/b)^2} \qquad (8)$$

The depolarization factors for a sphere (a/b=1) are N (a, b, c)= 1/3, 1/3, 1/3.

The formation factor is an intrinsic property that remains constant with varying fluid conductivity. In saturated conditions the intrinsic formation factor is the same as the apparent formation factor.

The second empirical equation that is called second Archie’s law can be written as:

$$ECa = ECw\,.\varepsilon^m.S^p \qquad (9)$$

Where S is a saturation degree; p saturation index with a value for sand and silt estimated as 2 and 1.98 respectively (Cosentini et al., 2012). The saturation index is usually larger than the cementation index (n>m), because as saturation decreases, the water films surrounding the grains become thinner and the conducting paths become more tortuous (lesmens and Friedman, 2005). For coarse-textured sands, the semi-empirical model of Mualem and Friedman (1991) predicts that m=1+L and p=2+L, where the tortuosity exponent L can be taken as 0.5 from Mualem’s (1976) model for predicting the soil-water-retention function parameters, making m=1.5 and p=2.5.

Slater (2007) has used effective porosity instead of porosity (ε). Waxman and Smits (1968) also proposed the above equation (5) who studied the effects of saturation on the electrical conductivity of oil-bearing shaly sandstones.

Archie’s law in constant porosity and water salinity conditions is:

$$\frac{ECa}{Ecw} = S^p \qquad (10)$$

The Kozeny and Carman, or K-C equation(Carman, 1939), can be expressed as:

$$ks = \frac{1}{aFS_p{}^n}; p = 2 \qquad (11)$$

Where ks, Sp and a are the hydraulic permeability, specific surface area and tube shape factor (a dimensionless number between 1.7 and 3)

Purvance and Andricevic (2000b) derived a linear log–log empirical relation between K and ECa (Slater, 2007):

$$K = a(ECa)^b \qquad (12)$$

The relationship between formation factor (FF) and hydraulic conductivity takes the form (Mazac and Landa 1979):

$$K = a(FF)^b \qquad (13)$$

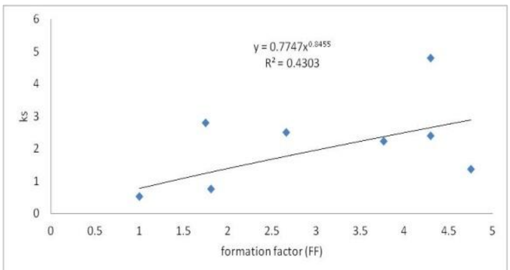
In the last two equations (12 and 13), a and b are fitting parameters.

Two hypotheses for 0-50 cm of soil depth data were tested:

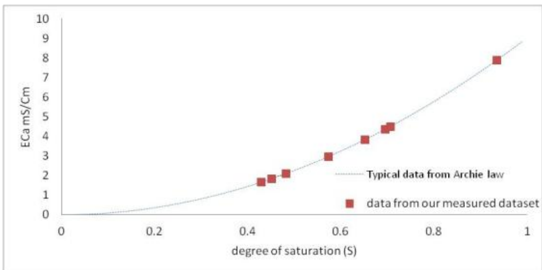
H0 (1), assume that the maximum measured ECa correspongs to the saturated soil bulk (soil solution) EC and derive FF from Eq. (5); there is no relationship between soil moisture, EC and effective formation factor levels and Ks; parameters a (0.7747) and b (0.8455) of empirical equation 13 were derived from Ks plotted vs FF (fig 4 a). Afterwards by assuming a constant porosity and water salinity of the soil, the degree of saturation can be calculated with equation 10. Results of this step has been compared to typical first Archie's law (fig 4 b). Finally, predicted Ks is compared with measured Ks (fig 4c).

H0 (2), assume a saturation condition, derive the maximum measured EC or saturated soil bulk (soil solution) EC with second Archie's law, (equation 9); there is no relationship between soil moisture levels and EC. Using equations 7 and 8, m was determined as 1.5, and by assuming tortuosity index equal to 1, FF was calculated based on eqation (6). Measured Ks was plotted vs FF and the parameters a and b from the empirical equation 13 were derived (fig 5a). Finally, measured Ks is plotted vs predicted Ks (Figure 5b).

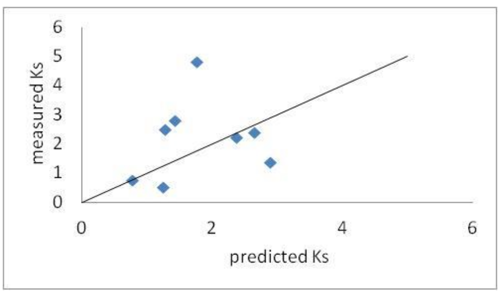
The result of the first and second hypothesis are shown in figures 4 and 5. Both approaches were acceptable based on the available data. New data are needed to further validate this.



a)



b)



c)

Figure 4. Relations between Ks (cm/h) and FF (a), and ECa (mS/cm) and S (b) for the top 50 cm of soil and measured Ks vs predicted Ks (c) based on relation between Ks an FF under first hypothesis H0(1).

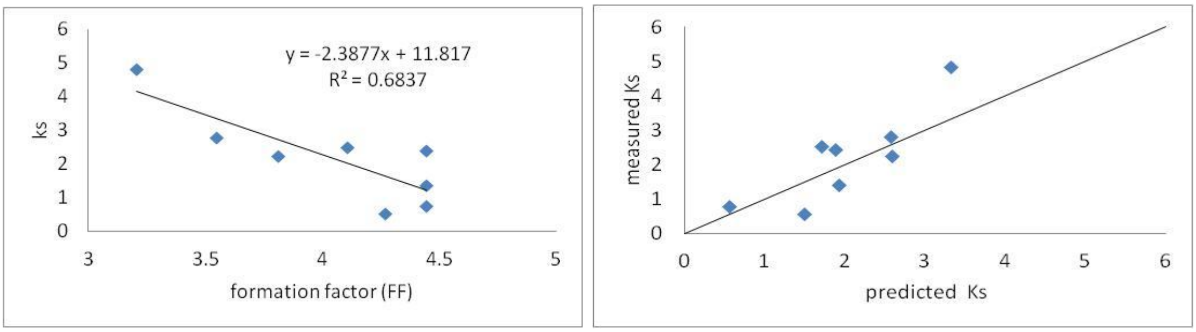


Figure 5. Relations between Ks and FF, and measurd Ks vs predicted Ks based on relation between Ks an FF under second hypothesis H0(2).

2.2: Scientific in- and output

Courses and workshops

- Aquacrop workshop from Monday 16th to Friday 20th July 2012 at KU Leuven University, by Dirk Raes
- ENVITAM course on HP1 (HYDRUS + PHREEQC). From 25th to 28th March 2013 at Gent University (Faculty of Bioscience Engineering), by Diederik Jacques.
- Contaminant transport in soil, second semester 2012-2013, Gent University, by Prof. Piet Seuntjens
- Soil physics, first semester 2012-2013, Gent University (Faculty of Bioscience Engineering), by Prof. Wim Cornelis
- Land information system, second semester 2012-2013, Gent University (Faculty of Bioscience Engineering), by Prof. Ann Verdoodt
- Intermediate academic English course, first semester 2012-2013, Gent University, by university language center (UTC)

Publications

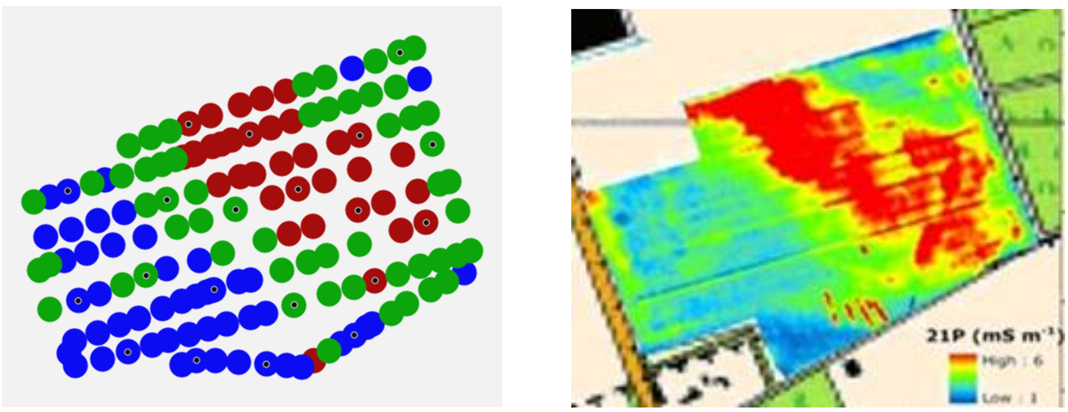
- Rezaei, M., P. Seuntjens, I. Joris, W. Boënne, W. Cornelis (2013). Estimation of hydraulic properties in a two-layered sandy soil for irrigation management purposes, in preparation.

Chapter 3: Future perspectives

3.1 Evaluation of the results and currently missing elements

The dataset now consists of data for two growing seasons and will be kept up-to-date for the next years for validation of our results. Monitoring equipment in the field will be checked for performance regularly. We will install new sensors in the field for two or three repetitions at locations or other places (higher accuracy of measurement and avoid ill-posed optimization).. Selection of the best location to install new sensors (soil mositure probes and tensiometers) in the field will be part of the research plan for next year.We will derive a groundwater depth for the field based on the DEM (digital elevation model) and check this with measurements of groundwater depth in the field.

Two hypotheses for the purpose of estimating the soil hydraulic properties from the field were investigated. So far no hypothesis could be rejected and we need new data to validate and finalize the results. Therefore additional sampling will be conducted. To this respect, a design-based and model-based sampling strategy was investigated. A user-friendly software package (ESAP) developed by Lesch et al. (2000), which uses a response-surface sampling design, has proven to be particularly effective in delineating spatial distributions of soil properties from ECa survey data (Corwin and Lesch, 2005). The ESAP model was used for a full sample design (20 locations). For the model based sampling design the Fuzzme software (Minasny, and McBratney, 2002) was used to classify the ECa field data set. According to the results, a classification using 3 classes came out best. The interesting result was that the suggested 20 locations from the ESAP model (design-based approach?) exactly cover the three classes of Fuzzme output (model-based approach?). Therefore the model-based sampling strategy (ESAP model) was chosen and soil sampling and field Ks measurements will be conducted in the next step. Figure 6 shows the map of the classified site with Fuzzme and the 20 soil sampling locations with the ESAP software.



a) b)

Figure 6. a) Field site classified with Fuzzme software (red, green and blue circles) and 20 sampling locations from ESAP software (black dots) and b) ECa map (0-100cm) of the field (from www.orbit.ugent.be).

We will futher investigate the correlations between ECa data and hydraulic properties. Additional measurements of Ks in the field will allow to find and validate a relationship between soil properties and the apparent electrical conductivity (ECa), measured by the

EM38DD sensor. This way, a spatial distribution of Ks for the whole field can be derived. In this respect, a sampling design is developed using a model ESAP where soil samples will be taken (fig 6) and soil physical properties will be measured (in the field and lab).

Sensor readouts will be fed to the Hydrus models and water flow in the plant root zone will be calculated. When new measurements become available they are assimilated in the model to further optimize the model parameters and to improve the model predictions. The improved model predictions will be used to activate or deactivate the irrigation, based on the plant requirements, chemical composition of solution and the climatological conditions. The irrigation can be optimized using optimization algorithms using predefined criteria in terms of minimal water use and maximal growth.

In a further modelling set-up, quasi 3D-modelling of water flow at the field scale will be conducted. The field will be modeled as a collection of 1D-columns representing the different field conditions (combination of soil properties, groundwater depth, root zone depth The data set of predicted Ks and other soil properties for the whole field constructed in the previous steps will be used for parameterising the model.

3.2 Planning

The literature study will situate the research in scientific literature. During the execution of the research plan, literature searches will be carried out for all of the different topics. This may lead to changes in the work plan during execution. Reporting will be done to Ghent University, Vito and the Ministry of science, research and technology of Iran. Below is a work schedule for the four year period (table 6).

Table 6: Overview of working schedule

<Meisam Rezaei> Started on <15.02.2012>		Actualised working schedule on **<23.5.2013>**			
	Tasks and parts of tasks	**YEAR 1**	**YEAR 2**	**YEAR 3**	**YEAR 4**
Task 1	**Literature Review, existing data analysis and work plan**				
	literature review: models, processes, inverse modeling, data assimilation methods, ECa, Penetrometer.....................				
	data analysis existing data field site at Vandenborne				
	GIS analysis field data and point-to-field extrapolation of hydraulic properties (in collaboration with UGhent)				
	Finding relationship between soil properties and available data (correlation and regression)				
	completing proposal writing work plan				
Task 2	**Parameter estimation and model calibration**				
	manual calibration of historical data set				
	inverse optimisation using Hydrus				
Task 3	**Modelling**				
	setup 1D hydrological models for individual soil columns				
	root distribution, plant uptake and ET- Crop based modeling				
	setup quasi 3D hydrological model (parallel columns) for the field site at Vandenborne				
	Application of data assimilation tools to sensor data Include weather forecast in predictions on water flow				
Task 4	**Field work and additional collection of data**				
	Installation of new sensor				
	Checking the data set and equipments twice to four times a month				
	Soil description and delineation of groundwater depth- soil sampling				
	Laboratory analysis				
Task 5	**Reporting**				
	Draft paper on the modelling.......,				
	Draft a paper on penetrometer data and ECa data set				
	take a note and writing a draft of thesis.				
	Journal and conference paper				
Task 6	**Doctoral education**				
	Course on Contaminant Transport in Soil, Physical Land Resources, Soil Physics, Land information system				
	English language and writing course				

Legend: (The vertical green line indicates the end of the present quarter)

Planning starting doctorate   Finished   Not planned, additional quarters   Planned but not realised

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