Constructing and optimising a parsimonious groundwater recharge model using neutron probe data.

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Abstract: Simulating the actual groundwater recharge rate of groundwater models is often a difficult procedure and is usually determined from an inverse method based on observations of water table depth alone. However, when studying land use change, it is necessary to understand how the local unsaturated zone controls recharge rates. The complicating factors of soil heterogeneity and macroporosity effects are difficult to represent in a physical-based model of the unsaturated zone. However, it is possible to observe soil moisture patterns across the unsaturated zone across space and time using Neutron Probe (NP) data. This can be done in-situ and under a range of land uses. Whilst it is appreciated that NP data can have its own errors and does not actually depict the recharge rate itself, it does give valuable information of unsaturated zone soil moisture activity. Equally, the physical processes of unsaturated zone activity, although well established, in the Mualem-van Genuchten (MVG) equations, are themselves quite complex with parameters that are difficult to determine *a priori*. Here, this paper shows two techniques for addressing these problems. The first analysis will clearly show that a number of the MVG parameters can be fixed without affecting the recharge rate of the model, this gives rise to a simplified model called the Simplified MVG (SMVG). Secondly, an inverse optimisation technique is proposed that capitalises on the observed NP soil moisture profile data which minimises soil heterogeneity and NP errors effects by 'smoothing' moisture fluxes across multiple soil layers. The technique gives a physical-based origin to the SMVG model parameters even though the soil output hydraulic conductivity profile model uses 'effective', optimised parameters. The method proposed can capitalise on field observation and may allude to even better hydro-geophysical data measurements that can be used to establish a simple, field characterisation technique to understand the groundwater recharge term across space.

Keywords: *Recharge; Unsaturated; van Genuchten soil parameters; Heterogeneity; Inverse modelling*

1. INTRODUCTION

To predict the impacts of land use change (such as afforestation and defforestation) on recharge, it is vital that in-situ unsaturated zone measurements are made beneath the specified land units. Thus, the soil parameters that describe the unsaturated hydraulic conductivity, need to be known accurately, and must reflect the soil heterogeneous effects.

The unsaturated hydraulic conductivity is often determined from measurements of soil hydraulic properties, alone. However, these methods are not totally satisfactory, for example, Van Genuchten and Nielson (1985) and by Luckner *et al.* (1989), show that the measurement of the saturated hydraulic conductivity from soil samples, does not pick up the overall flow such as macropore flow.

To overcome this problem, the soil parameters that are needed to determine the unsaturated hydraulic conductivity, must be performed in situ, in a non-destructive way, in order to pick up all the key recharge processes, for example bypass flow. At this time, in-situ NP well logging is a suitable method for this task, see Chapellier (1992). Thus it should be possible to determine the unsaturated hydraulic conductivity as a function of depth, for each NP well logging location. As such time series measurements of the soil moisture profile, can give repeat patterns across a range of wet and dry periods.

To pursue this methodology, one must be able to approximate the recharge rate inferred by the time series of observations using an accepted physical basis. This must then be followed by a robust optimisation technique for determining the key recharge parameters across the soil profile.

The first step is to verify that the Mualem-van-Genuchten model (MVG) can be used to determine the unsaturated hydraulic conductivity using soil moisture measurements alone. Also, an investigation of the model is carried out to test if the model can be simplified without affecting the recharge.

The second step is to develop a scheme that enables the determination of the unsaturated hydraulic conductivity for every layer. There are complications due to the fact that optimising the layers sequentially for highly heterogeneous soil produces poor results. The heterogeneity is described by using a technique that employs the average time series soil moisture, and then the remaining soil parameters are optimised by using a special scheme in order to produce a good agreement between the simulated and observed soil moisture as shown in Figure 1. In Figure 1, the 40 soil layers are well reproduced for the dry and wet period, by only optimising 2 MVG parameter per layer, and 2 parameters to represent the heterogeneity for the whole column.

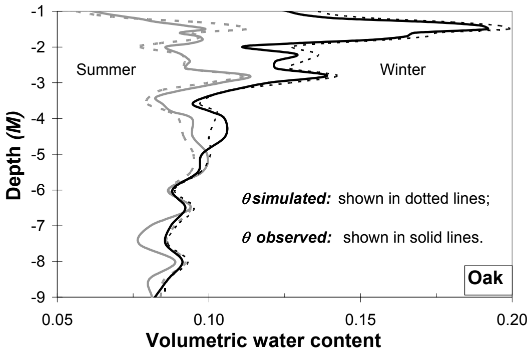

Figure 1. Snap shot of the observed and simulated soil moisture, for the driest and the wettest period for Oak forest.

2. THE MUALEM-VAN GENUCHTEN MODEL

2.1. The equations

The soil moisture retention curve can be obtained from van Genuchten (1980):

$$Se = \frac{\theta - \theta res}{\theta sat - \theta res} = \frac{1}{\left[1 + (\alpha . h)^n\right]^{1-\frac{1}{n}}} \tag{1}$$

where *Se* is the relative saturation, the parameters θres and θsat are respectively residual and saturated water contents, where θ is volumetric water content (L^3L^{-3}), with $\theta res < \theta < \theta sat < 1$, α (> 0) is related to the inverse of the air entry pressure (L^{-1}), and n (> 1) is a measure of the pore-size distribution (-).

Mualem (1976) and van Genuchten (1980) described the unsaturated hydraulic conductivity function with the Malem-van-Genuchten model (MVG):

$$K(Se) = Ko.Se^l . \left[1 - \left(1 - Se^{\frac{n}{n-1}}\right)^{1-\frac{1}{n}}\right]^2 \tag{2}$$

where *K(Se)*, is the unsaturated hydraulic conductivity ($L\ T^{-1}$), *Ko* is a optimised saturated hydraulic conductivity ($L\ T^{-1}$), and l (-) is a shape factor *(l >0)*.

Ksat is denoted to be the physical value of the saturated hydraulic conductivity ($L\ T^{-1}$).

2.2. The 'non physical' soil parameters.

The six soil parameters of the MVG model are: $\theta sat,\ \theta res,\ Ko,\ n,\ l,\ \alpha$. Kosugi (1999) and Hoffmann-Riem *et al.* (1999) concluded that the soil parameters should not be interpreted as true physically meaningful parameters but as empirical shape factors. The study found that *Ko = Ksat* and *l=0.5* leads to very poor prediction of the unsaturated hydraulic when compared to optimised *Ko* and *l* values. Consequently the soil parameters determined from inverse modelling are been treated as non physical effective parameters. Thus the finding of this paper, argue that effective values of the *K(Se)* relationship can be found for any monitored location.

3. SIMPLIFING MVG MODEL

3.1. Simulating a physically based recharge model : SHELUC

SHELUC recharge model (System Hydrologique European Land Use Change model) developed in Newcastle, is a physically-based hydrological model that uses both the MVG model and the Richards equation. As such it can be used to create multiple simulation outputs that can be analysed to find out the sensitivity and operation of the MVG parameters. Thus, any range of soil types and wetting and drying scenarios can be tested.

A more detailed description of SHELUC is thoroughly described in (Parkin *et al.,* 2003).

3.2. Rationale for fixing *Ko* and *l*

Using MVG model simulations it was shown that *Ko* was not sensitive for the determination of *K(Se).* When *Ko* is kept constant and the other soil parameters are optimised, negligible changes to *K(Se)* relationship was encountered for all ranges of soils. The only condition to be satisfied is that $Ko \geq Ksat$. If equation 2 is written as:

$$K(Se)= Ko.\ Se^{l}.\ Function(Se) \tag{3}$$

By inspection $Se \leq 1$, $l > 0$ and $Function(Se) \leq 1$. Since the soil parameters are taken as 'non physical', the soil parameters used to describe $Se^{l}.\ Function(Se)$ are optimised to a value between 0 and 1.

It is found, that by keeping l constant and set equal to 1, also makes negligible difference to the overall *K(Se)* relationship. The soil optimised effective parameter, *Function(Se)* will adjust itself for any variation in the 'physical' value of l .

The simplification of fixing l =1 and $Ko \geq Ksat$ is denoted as the Simplified Mualem van Genuchten model (SMVG).

3.3. Method to show the redundancy of *Ko* and *l*

To validate the universality the SMVG model, different tests are been performed to show that there are negligible differences for all soils types between *K(Se)* relationship of the SMVG model and the MVG model.

The soil parameters of the MVG model are tested for sand, loam, silt and clay soils. The soil parameters were derived from 235 soil samples from the international UNSODA database (*Leij et al.,* 1996). The values of the soil parameters are found in Table 1.

Table 1. Average soil parameters for each soil texture group determined from the UNSODA database.

	θres (-)	θsat (-)	n (-)	l (-)	Ko (cm.d^{-1})
Sand	0.052	0.396	2.233	1.29	173
Loam	0.056	0.512	1.191	1.42	107
Silt	0.031	0.428	1.377	0.82	50
Clay	0.098	0.512	1.300	0.26	20

The soil parameters of the SMVG model that are been optimised are θsat, θres and n. It was found that the arbitrary given value of $Ko= 400\ cm.\ d^{-1}$ for all soils gave excellent agreements. The parameter l is set equal to 1 in all simulations. The results are shown in Figure 2.

3.4. The results of fixing *Ko* and *l*

The agreement between SMVG and MVG as shown in Figure 2 are accurate for the complete range of soil textures in the UNSODA database. It can be concluded that SMVG can be used instead of the MVG with confidence for all range of soils types, the only condition is that $Ko \geq Ksat$.

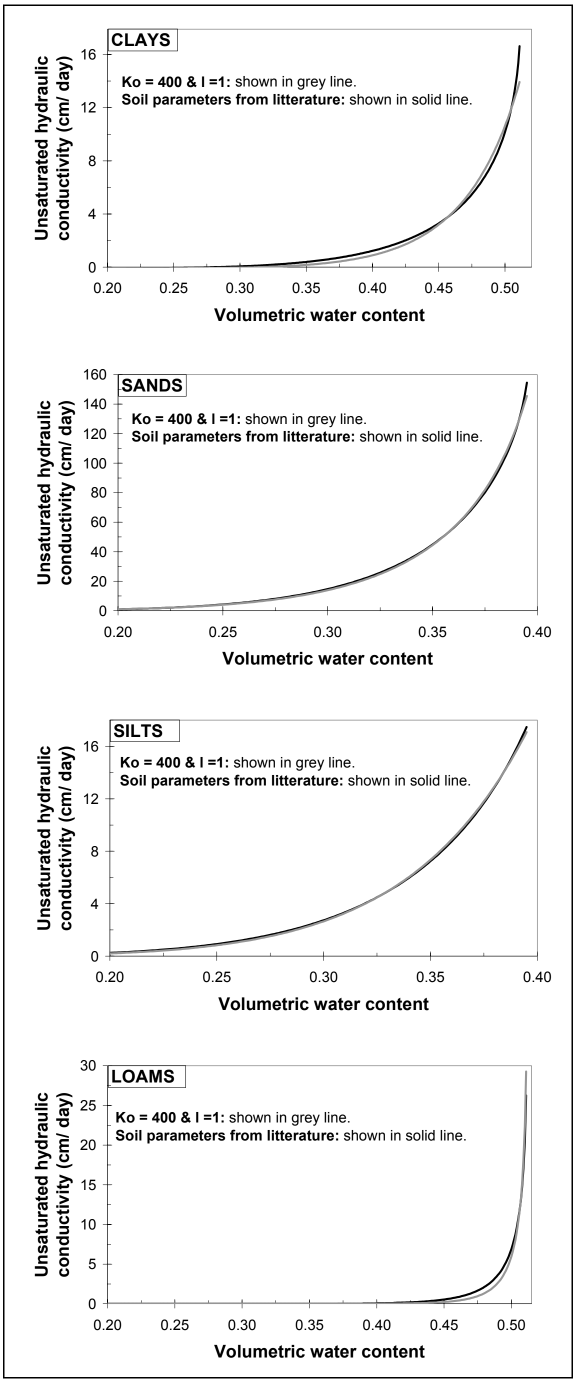

Figure 2: For each soil textural the *K(Se)* relation is plotted for the MVG and the SMVG model. The agreements are excellent.

3.5. Rationale for fixing the *n* parameter

Surprisingly, it was found that by optimising the remaining soil parameters θres, θsat, α against the SHELUC recharge model simulations, that no differences in recharge were encountered when *n* was kept fixed throughout the soil profile. In the current study the data that is presented in Figure 1, is for a sandy soil. This means that only a small portion of *K(Se)* relationship has been tested, thus facilitating α to compensate for any fluctuation of *n*. This is well illustrated in Figure 3, where the 3 log *K(Se)* relationship for *n* equal respectively to 1.4, 1.6, 1.7 are plotted. Curiously the 3 plots meet at one point that is the average of the observed time series soil moisture, $\overline{\theta obs}$ (L^3L^{-3}). In this case study the variance of θobs is small.

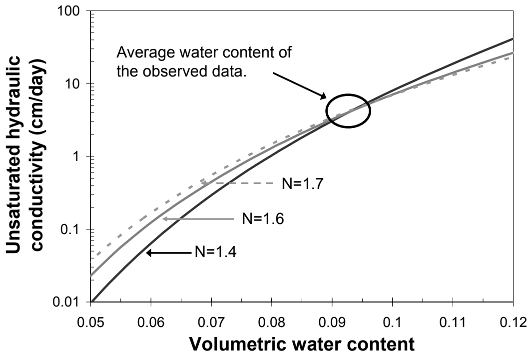

Figure 3 represents *K(Se)* relationship for the SMVG model with *n* being fixed. N.B. the 3 plots cross at $\overline{\theta obs}$.

No differences in recharge were encountered if *n* was kept constant for dry or wet soils (the variance of θobs is small). However, it seems very unlikely that *n* can be kept constant for soils experiencing extreme conditions, (that is where the variance of θobs is high*)*.

4. THE PROBLEMS CAUSED BY HETEROGENEITY

Figure 4, shows the impact of heterogeneity effects on the soil moisture profile. The two main reasons for the discrepancy in soil moisture pattern are:

- Errors caused by the inaccuracy of measuring highly heterogeneous soil with sharp discontinuous boundaries;
- The inability of the flow models to handle rapid changes in water content.

4.1. Removing the redundant heterogeneity effects from the observed data sets

In the calculation of recharge the change in soil moisture $\Delta\theta_j$ is more important then the actual value of θ_j in each layer. Thus by plotting $\Delta\theta$ instead of θ, the "true" heterogeneity effects can be studied. When $\overline{\Delta\theta_j}$ across layers are different to the overall pattern, then the heterogeneity layering effect is either:

- A faulty calibration curve that transforms raw NP data into the observed θ value, (for example, the calibrated curve may be different for clay layers as for stony);
- The soil moisture profile pattern and water movement caused by bypass flow.

Ideally these anomalies need *a priori* correction. However, the current method can correct for any anomaly within the automatic optimisation scheme. This is achieved by smoothing across soil layers reflecting the transmission of water from one layer to another.

Thus an a-priori improvement to acquiring accurate soil moisture profiles is desirable. However, the smoothing optimisation function, using the SMVG model does resolve apparent movements in water that eventually impact upon the groundwater recharge term.

5. A SIMPLE METHOD TO REDUCE THE HETEROGENEITY EFFECTS

5.1. Introducing the problem

In order to quantify recharge under heterogeneous soil by using the Richards' equation, *K(Se)* is estimated for every layer by using the SMVG model with *n* kept constant for the whole profile. The soil parameters are calibrated against SHELUC model simulations, such that for every layer the simulated soil moisture θsim_j (L^3L^{-3}) is matched with θobs_j as shown in Figure 1. In our case study θobs_j is monitored up to a depth of 9m and the soil column is divided into 40 layers (*j*=1 to 40). There are 3 remaining soil parameters to be optimised (θres_j, θsat_j, α_j) per layer *j*, resulting in a total of 120 soils parameters to be optimised.

5.2. Reducing the number of soil parameters to be optimised

Here is presented a simple method that determines θres_j for each 40 layer with just 2 soil parameters θres_{mult}, θres_{shift} (-). The property used is shown in Figure 4. The average soil moisture for each layer, $\overline{\theta obs_j}$ (L^3L^{-3}) gives detailed information about the lithologocal effects. In the profile there are high $\overline{\theta obs_j}$ (-1,5m and -3m) representing layers that are wetter, due to local slow percolation and lower *K(Se)*. These layers are known to contain a greater percentage of clay. On the other hand in the profile there are lower $\overline{\theta obs_j}$ (-1m, -2m and -3m) representing layers that are drier, due to water moving faster due to higher *K(Se)*. These layers are known to contain a higher percentage of pebbles.

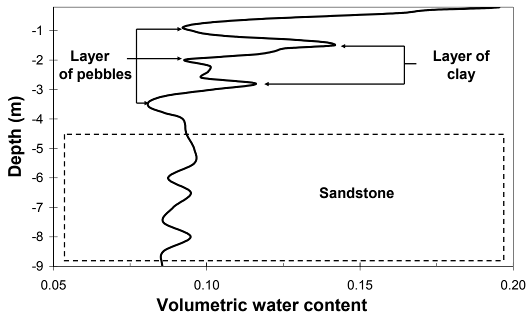

Figure 4. The average time series soil moisture for every layer over a period of 3 years $\overline{\theta obs_j}$ for the oak site, reflecting information on the heterogeneity.

θres_j is computed for the 40 layers by using the following equation:

$$\theta res_j = \theta res_{shift}.\overline{\theta obs_j} + \theta res_{mult}.\left(\overline{\theta obs_j} - \overline{\theta obs}\right) \qquad (5)$$

The limitation of the current method is that to determine the lithological effects successfully, one needs at least a dry and wet period.

5.3. Optimising the 40 layers

It was found that optimising each layer separately one by one produces poor results, therefore a strategy to optimise the 80 soil parameters simultaneously is presented.

The origin of poor results invariably due to macropore flows and lenses of clay and pebbles (as shown in Figure 4). Thus optimisation that isolate each layer without considering the overall water movement causes unrepresentative parameters and thus poor overall recharge results. Therefore when optimising the profile soil parameters, one must consider firstly, the whole profile at the same time. Secondly, grouping local layers (or zones) together can successively address both heterogeneous patterns and identify an effective unsaturated zone value for those layers.

The simple solution to this problem is to optimise the different layers in a specified order and pattern as shown in Table 2. The "*order of optimising the layers*", in Table 2, represent the different sequence of optimising the different layers. The 9m profile is divided in to 40 layers or cells. The grey boxes in Table 2, show the grouping of different layers in which the soil parameters have got the same optimum value. In the first step, all the layers have got the same optimum soil parameters ($\theta sat_1 = \theta sat_{40}$ and $\alpha_{1} = \alpha_{40}$). In the second step only the upper root zone is optimised, and then the third step operates on the deeper intermediate zone. It was found that optimizing from top-to-bottom produces better simulation result. The root zone is split into 2 zones, and then the intermediate zone is split into 2 parts and the optimisation is repeated.

Table 2: Represents the order of optimization the different groups of layers. In this particular case the root zone is set to be 2m.

Depth	ORDER OF OPTIMISING THE LAYERS																						
(m)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
0.1	■	■		■				■								■							
0.2	■	■		■				■								■							
0.3	■	■		■				■									■						
0.4	■	■		■				■									■						
0.5	■	■		■				■									■						
0.6	■	■		■					■									■					
0.7	■	■		■					■									■					
0.8	■	■		■					■										■				
0.9	■	■		■					■										■				
1.0	■	■		■					■										■				
1.1	■	■			■					■										■			
1.2	■	■			■					■										■			
1.3	■	■			■					■											■		
1.4	■	■			■					■											■		
1.5	■	■			■					■											■		
1.6	■	■			■						■											■	
1.7	■	■			■						■											■	
1.8	■	■			■						■												■
1.9	■	■			■						■												■
2.0	■	■			■						■												■
2.2	■		■			■						■											
2.4	■		■			■						■											
2.6	■		■			■						■											
2.8	■		■			■						■											
3.0	■		■			■						■											
3.2	■		■			■							■										
3.4	■		■			■							■										
3.6	■		■			■							■										
3.8	■		■			■							■										
4.0	■		■			■							■										
4.5	■		■				■							■									
5.0	■		■				■							■									
5.5	■		■				■							■									
6.0	■		■				■							■									
6.5	■		■				■							■									
7.0	■		■				■								■								
7.5	■		■				■								■								
8.0	■		■				■								■								
8.5	■		■				■								■								
9.0	■		■				■								■								

■ Layers to be optimised together

The maximum amount of splitting depends on the severity of the heterogeneity in the profile. In the case study significant improvements in the matching of the θobs to θsim were achieved until the 6th step of splitting and well before the layers required individual optimisation.

6. CONCLUSIONS

Mualem-van-Genuchten model is well suited to determine the unsaturated hydraulic conductivity accurately when an inverse method is proposed.

However, the optimum soil parameters must be treated as non physical effective values. It has been demonstrated through SHELUC recharge model simulations and through sensitivity analysis of Mualem-van-Genuchten model that a simplified MVG model exists for all soils types with out altering the unsaturated hydraulic conductivity profile and recharge estimates. Equation 2 is thus simplified by removing the shape factor *l*, and by fixing the saturated hydraulic conductivity *Ko* to a value higher then the expected value.

For sandy dry soils, it was found through runs of SHELUC recharge model, that no difference in recharge was encountered when the soil parameter *n* is kept constant. There is some evidence that this can be generalised for soils having small range of soil moisture.

A straightforward robust scheme has been developed to simulate highly heterogeneous soils profiles, by fitting the 3 soil parameters (θres_j, θsat_j, α_j) for each per layer. However θres was not optimised per each layer, instead an equation was developed that uses two optimum parameters per layer. The pattern of soil profile water movement and the effects of the heterogeneity is abstracted from knowledge of the average soil moisture profile. Subsequently a simple technique has been developed to optimise the 80 remaining parameters, in order that the overall simulated soil moisture gives a good match with the observed time series soil moisture profile.

The ability to use a simplified MVG model, when used in tandem with observed soil moisture profile data, gives a good insight to recharge estimates under a range of land uses. The procedure creates an effective unsaturated water movement model based on effective parameters derived from the MVG. The ultimate accuracy of the method is dependent on the accuracy of the hydro-geophysical methodology used. Even if inaccuracies in the method are present, there is still valuable information in the observations that can be analysed by using the optimisation, 'smoothing' process proposed here.

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