Modeling Soil Water Dynamics with Time-Variable Soil Hydraulic Properties

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Abstract: Modeling soil water dynamics requires an accurate description of soil hydraulic properties, i.e. the retention and hydraulic conductivity functions. Generally, these functions are assumed to be unchanged over time in most simulation studies. However, there is extensive empirical evidence that soil hydraulic properties are subject to temporal changes. In this paper, we implemented temporal changes in the soil hydraulic properties in a Richards' equation simulation of soil water dynamics. Based on repeated measurement data of the soil water retention curve over a vegetation period, we compared the impact of using constant vs. temporally changing hydraulic functions on water flow simulation for different tillage methods. We observed distinct differences in the soil water content between the simulations for all tillage methods. The results show the remarkable effect of time-variable retention parameters on the soil water dynamics for tilled and non-tilled top soils.

Keywords: Soil hydraulic properties, timevariable modeling, Kosugi retention model, soil tillage, pore-size distribution

1. Introduction

For many applied questions in the fields of crop production and agronomy, soil water dynamics are of fundamental importance. Modeling can be a valuable tool to optimize its management (Roger-Estrade et al. 2009). However, such soil water modeling requires an accurate description of soil hydraulic properties, i.e. the soil water retention characteristics (WRC) and hydraulic conductivity functions. Generally, these constitutive functions are assumed to be unchanged over time in most simulation studies. For example, the widely-used simulation software HYDRUS (Šimunek et al. 2006)

enables the solution of unsaturated media flow problems with different spatial WRC definitions, but it still does not account for time dependent soil retention characteristics. However, there is extensive empirical evidence that soil hydraulic properties are subject to temporal changes particularly in the near-saturated range where soil structure essentially influences water flow characteristics (Daraghmeh et al. 2008, Or et al. 2000). Especially, the structure of soil top layers is subject to changes during time, caused by wetting and drying, solution composition agricultural operations, and biological activity (Leij et al 2002). For instance, soil tillage is used to improve soil structural properties by changing the soil pore-size distribution (PSD). Since these modifications are quite unstable over time, the PSD, expressed by its median pore radius, decreases after tillage (Leij et al 2002). This effect should be largest for conventional tillage (CT), were the soil is ploughed after harvest every year.

Many functions for expressing the WRC have been published (e.g. Brooks and Corey 1964, Van Genuchten 1978). They are compatible with models that describe the relative hydraulic conductivity of soils (e.g. Burdine 1953, Mualem 1976). However, most of these models are empirical curve-fitting equations and do not base on physical fundamentals (Kosugi 1994). In contrast, the soil retention model of Kosugi (1994) bases on the lognormal distribution of the soil pores as described by the Laplace-Young equation (Leij et al. 2002).

In this study, we implemented a water flow model using the Earth Science Module in COMSOL Multiphysics, that accounts for time variable retention characteristics in the uppermost soil layer. The effect of time dependent changes of the WRC on soil water dynamics, as expressed by the volumetric water content, was tested and evaluated for different tillage systems.

2. Governing equations

Water flow in unsaturated or partly saturated soils can be described with the Richards' equation (Richards 1931):

$$C\frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left(K \frac{\partial h}{\partial z} - K \right) \quad (1)$$

where *h* is the soil water pressure head or water potential (dimension L), *t* the time (T), *z* the soil depth (L), *K* is the hydraulic conductivity (LT⁻¹) and *C* is the soil water capacity (L⁻¹). *C* is defined by the slope of the WRC ($d\theta/dh$), where θ is the volumetric water content of the soil (L³ L⁻³). In the present study, the WRC in the upper soil is described by Kosugi's lognormal retention model (Kosugi 1994):

$$\theta(\mathbf{h}) = \begin{cases} \left\{ \frac{1}{2} \operatorname{erfc} \left[\frac{\ln(\mathbf{h}/\psi)}{\sqrt{2}\sigma} \right] + \theta_{\mathrm{r}} \right\} & (2) \\ \cdot (\theta_{\mathrm{s}} - \theta_{\mathrm{r}}) & (\mathbf{h} < 0) \\ \theta_{\mathrm{s}} & (\mathbf{h} \ge 0) \end{cases}$$

where ψ (L) and σ are parameters that change the shape of the retention curve, θ_r is the residual volumetric water content and θ_s is the water content at saturation. The effective saturation S_e is defined as follows (Kosugi 1994):

$$S_{e}(h) = \frac{\theta(h) - \theta_{r}}{\theta_{s} - \theta_{r}}$$
 (3)

Applying Mualem's model, the unsaturated or relative hydraulic conductivity K_r is defined as follows (Kosugi 1994):

$$K_{r}(\theta) = \begin{cases} K_{s}\sqrt{S_{e}} \cdot \left(\frac{1}{2}\right)^{2} & (4) \\ \cdot \left[\operatorname{erfc}\left(\frac{\ln(h/\psi)}{\sqrt{2\sigma}} + \frac{\sigma}{\sqrt{2}}\right) \right]^{2} & (h < 0) \\ K_{s} & (h \ge 0) \end{cases}$$

As mentioned above, the specific capacity C is defined as the derivative of the WRC:

$$C = \frac{d\theta}{dh} = \frac{\left(\theta_{s} - \theta_{r}\right)\psi^{2}}{\sqrt{2\pi\sigma h}}$$
$$\cdot \exp\left(\frac{\ln\left(h/\psi\right)}{\sqrt{2\sigma}}\right)^{2} \quad (5)$$

According to Leij et al. (2002), the PSD can be obtained with a similar equation:

$$f(r) = \frac{\left(\theta_{s} - \theta_{r}\right)}{\sqrt{2\pi\sigma r}} \exp\left(\frac{\ln\left(r/r_{m}\right)}{\sqrt{2\sigma}}\right)^{2} \quad (6)$$

where $f(L^{-1})$ is the frequency of a certain pore radius r(L). $r_m(L: \mu m)$ is the median pore radius that can be calculated from ψ (hPa) by $r_m =$ 1490/ $\psi \exp(\sigma^2)$ (Leij et al. 2002).

In the lower soil horizons, the WRC has been defined by the model of Van Genuchten (1978). Since the governing equations are already implemented in the Earth Science Module of COMSOL Multiphysics, they are not discussed in this paper.

3. Methods

Field measurements were accomplished on an arable field near the village of Raasdorf, Lower Austria, 20 km east of the city of Vienna. At this agricultural investigation side, the effects of different tillage methods, in specific conventional tillage (CT), reduced tillage (RT) and no-tillage (NT), are observed by our working group. The soil can be classified as a Chernozem with a sandy loam texture. For the different tillage systems the hydraulic properties of the uppermost soil layer (0-15 cm) have been determined by infiltration measurements with a tension-disc infiltrometer (Soil Measurement Systems, USA; diameter of the disc: 20 cm). Three replicate measurements were conducted for every type of tillage several times between August 2008 and July 2009 (Tab. 1). The adjusted hydraulic pressure heads were -10 cm, -4 cm, -1 cm, and 0 cm. Undisturbed soil samples were taken with steel cores (volume: 200 cm³) before and after each measurement to determine the initial and final volumetric water content below the infiltration disc gravimetricly. The software HYDRUS 1.10 (Šimunek et al.

tillage	date	day	θ_{s}	θ_{r}	$\mathbf{K}_{s} (\mathbf{m} \mathbf{d}^{-1})$	ψ (hPa)	σ	r _m (µm)
СТ	01.Aug.08	1	0.51	0.11	2.29	56.44	1.79	1.07
	23.Okt.08	84	0.51	0.11	2.78	21.15	1.34	11.76
	03.Dez.08	125	0.50	0.11	1.56	31.22	1.55	4.38
	01.Apr.09	244	0.43	0.11	1.00	41.32	1.68	2.13
	21.Jul.09	355	0.48	0.11	2.18	36.42	1.77	1.79
RT	01.Aug.08	1	0.53	0.11	1.14	9.28	1.19	39.11
	23.Okt.08	84	0.45	0.11	1.56	49.74	1.75	1.40
	03.Dez.08	125	0.50	0.11	0.33	29.29	1.61	3.83
	01.Apr.09	244	0.41	0.11	0.23	27.99	1.37	8.23
	21.Jul.09	355	0.49	0.11	0.68	27.98	1.59	4.27
NT	01.Aug.08	1	0.47	0.11	0.61	36.27	1.73	2.09
	23.Okt.08	84	0.43	0.11	0.12	34.40	1.54	4.04
	03.Dez.08	125	0.46	0.11	0.05	37.55	1.29	7.56
	01.Apr.09	244	0.43	0.11	0.10	39.46	1.44	4.77
	21.Jul.09	355	0.43	0.11	0.11	34.27	1.04	14.61

Table 1. Retention data of the upper soil layer as observed by infiltration measurements for the different tillage methods (CT: conventional tillage, RT: reduced tillage, NT: no-tillage). The date of the infiltration measurement, the day in the model, the volumetric water content at saturation θ_s , the residual water content θ_s , the saturated hydraulic conductivity K_s , the parameters of the Kosugi retention model, ψ and σ , and the median pore radius r_m are listed.

2006) was used to fit the retention model of Kosugi (1994) inversely to the infiltration measurements. As this paper focusses on the water movement modeling, the inverse estimation of the Kosugi parameter is not discussed in detail. The resulting parameters were used to calculate the PSD for every time of measurement.

The lower soil horizons were sampled with soil cores in depths of 40 cm and 70 cm and three replicates in July 2009. The WRCs of the subsoil layers were determined in the laboratory with a low pressure plate extractor (Soil Moisture Inc., USA) at pressure heads of 0.2, 0.5, 1.0, 2.0 and 3.0 bar. The program RETC (Van Genuchten et al. 1991) was used to fit the parameter of the Van Genuchten retention model to the observed data. For calibration of the model, measured data of the soil volumetric water content in different steps of depth were available over the modelled time.

4. Numerical Model

4.1 Model type and geometry

The soil water dynamics were simulated for a year (August 1st. 2008 to August 1st. 2009) on basis of the Richards' equation using the Earth Science Module of COMSOL Multiphysics 3.5a. Although the problem in priciple is one-dimensional, we chose a 2-D geometry for a

better illustration of the results. We used the transient pressure head analysis (esvr). As SI units were used, we changed the time step from seconds (s) to days (d) by changing the scalar variable gravity. The geometry was defined by a rectangle soil column with a width of 1.00 m and a depth of 1.20 m (Fig. 1). According to the observed soil horizons in the field, the geometry was devided into three subdomains: the upper soil from 0 to 0.15 m (tilled A-horizon, WRC determined by infiltration measurements), the lower part of the A-horizon between 0.15 m and 0.50 m, and the subsoil from 0.50 m to 1.20 m (C-horizon). The soil hydraulic properties of the lower subdomains were defined by the Van Genuchten retention model parameters. Since the time-dependent effect of tillage was expected to be negligible, we set the hydraulic properties to be constant in the lower soil horizons. To implement the retention model of Kosugi for the uppermost subdomain, we used the user-defined WRC definitions and the possibility to include functions written in MATLAB R2007b (The MathWorks Inc., USA).

4.2 Initial and boundary conditions

The model geometry was laterally confined by no-flux boundaries (Fig. 1). The lower boundary was defined by an unit gradient condition (*outflux* = $-K_r(h)$). On the basis of measured precipitation data, we used the empirical method



Figure 1. Model geometry and boundary conditions.

of Allen et al. (1998) to calculate the potential evaporation and transpiration. The precipitation and the evaporation, the latter reduced by a pressure head dependent reduction function, were applied to the model as upper boundary condition. Transpiration was implemented as sink term (*liquid source*) using a growth function and a reduction function according to Feddes et al. (2001).

Initially, the hydraulic pressure head h_0 was set to -0.5 m for the whole model geometry.

The Van Genuchten parameters of the A- and Chorizon were $\theta_s = 0.39$ and 0.41, $\theta_r = 0.10$ and 0.07, $K_s = 1.96 \text{ m d}^{-1}$ and 1.06 m d⁻¹, $\alpha = 3.05 \text{ m}^{-1}$ and 2.20 m⁻¹, and n = 1.19 and 1.24, respectively. To account for the WRC changing with time in the upper soil layer, adequate functions were fitted to the measured values for the Kosugi retention model parameters ψ and σ , the saturated hydraulic conductivity $K_{s,}$, and the soil water content at saturation θ_s (Tab. 1). For the simulations with constant hydraulic properties, median values for these parameters were used.

The accuracy of the implementation of the evapotranspiration was evaluated by a comparative simulation using HYDRUS. The model was calibrated with measured soil water contents. Calculations were made with constant and time variable retention parameters of the upper soil layer for all observed tillage systems.

5. Results and Discussion

5.1 Evolution of the pore-size distribution

The evolution of the PSD as determined by the infiltration measurements showed distinct differences between the applied tillage methods. As proposed by Leij et al. (2002), the PSD at the CT site shifted towards smaller pore sizes after mouldboard tillage (Fig. 2a, ploughing in mid-October 2008). Here, the change of the PSD is dominated by the agricultural operation. Compared to the other tillage methods, a quite high total porosity exists, as it is also expressed by the integral of the PSD, θ_s (Tab. 1). On the other side, the determined PSDs for RT (graph not shown) and NT (Fig. 2b) show a smaller shift during time and a lower total porosity. Moreover, the shift of the PSD is slightly towards larger pores. This effect might be caused by biological activities, such as earthworm burrows and plant root development (D'Haene et al. 2008).

5.2 Model implementation in COMSOL Multiphysics

On basis of the measured retention properties and precipitation data from the field site, we set up a water dynamic model in the COMSOL Multiphysics Earth Science Module sucsessfully. The initial and boundary conditions led to converging simulations for all variations. The implementation of the Kosugi retention model with MATLAB gave reasonable soil water contents. Due to the possibility to use timevariable retention parameters the model became very flexible, compared to classical simulation approaches. The results for the time course of the soil water content for time-constant retention properties agreed with comparative soil water simulations with HYDRUS (data not shown). In the subsoil, there was also a good agreement between modelled and measured soil water However, there were contents. distinct differences between measured and modelled soil water contents in the upper soil (data not shown). These differences, that have also been observed in the comparative simulation, will be subject of our future work.



Figure 2. Evolution of the PSD over time for a) conventional tillage (CT) and b) for no-tillage (NT). The PSDs were determined from the infiltration measurements according to Eq. 6.

5.2 Water dynamics with constant vs. timevariable hydraulic properties

For a better interpretation of the simulation results, we calculated the relative difference between the water contents with constant and with time-variable retention behaviour (Fig. 3b).

The results show distinct differences between the simulations for all methods of tillage. In the beginning of the simulated time (August – December 2008), we observed the most obvious differences in the soil water content, whereas in the later part of the simulation, these differences decreased. We trace this back to high volumetric



Figure 3. Simulation results. a) Volumetric water content θ in a depth of 10 cm simulated with time-variable soil retention properties for the different tillage systems (CT: conventional tillage, RT: reduced tillage, NT: no-tillage). b) Relative difference (%) between simulations of the soil water content with constant and time-variable soil retention properties. The asterisc (*) marks the mouldboard ploughing at CT in mid-October 2008. Note also the precipitation (mm) measured at the field site.

water contents in late autumn and winter in the upper soil, provided by a low evapotranspiration (Fig. 3a). As the simulation with time-variable hydraulic properties accounts for changes in the PSD, these structural changes affect the hydraulic behaviour most at high volumetric water contents. This result is in agreement with the findings of Daraghmeh et al. (2008). The results of the CT simulations show the effect of ploughing in mid-October impressively, as the retention potential decreases shortly after it. However, the effect of time-variable retention properties at lower soil water contents, as simulated in spring and summer 2009, seems to be negligible for CT. Noticeable differences for the other tillage methods occur mainly at high precipitation events and may be traced back to an underestimation of biological induced macropore-flow in the simulations with constant soil retention properties.

6. Conclusion and Perspective

As classical simulations of the soil water dynamics do not account for time-variable soil retention properties, we implemented a model approach with the Earth Science Module of COMSOL Multiphysics, that enables the flexible definition of these important control quantities. Using the MATLAB interface in COMSOL, the implementation of the Kosugi retention model allowed the definition of the soil retention properties strongly connected to the PSD of the soil. However, since now we used only empirical fitted functions for the time-variable retention parameters. A challenge for our future work will be the adaptation of a suitable PSD-evolution model, as proposed by Or et al. (2000) on basis of the measured data.

7. References

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