Simulation of evapotranspiration and drainage from potash tailings covers using Hydrus-1D

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Abstract: Evapotranspiration is the sum of evaporation of water from soils and transpiration from plants. It is a crucial part of the water cycle and can be measured using lysimeters. However, lysimeters require high maintenance and operation costs; as such, evapotranspiration models are used for making predictions. Thus, the aim of the present study was to calibrate the Hydrus-1D to predict the water balance components of a thin evapotranspiration covering layer for potash tailings piles. Further simulations were performed using different fine fraction proportions, soil textures and crop parameters. A high association between the calibrated and observed drainage of substrates was found, with a variation of 2.9% (approximately 13.6 mm). Drainage estimates were lower with increasing root depth, crop height and proportion of fine particles (< 2 mm diameter) in the substrates. Fine fractions in the substrates increased the water storage and the evapotranspiration capacity of the substrates and therefore contribute to improving the efficiency of evapotranspiration covers and can facilitate reducing brine drainage from potash tailings piles.

Keywords: water fluxes, greening, mining, perennial grasses, municipal wastes, coal combustion residues

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1 Introduction

Brine drainage from potash tailings piles impacts natural ecosystems due to the high concentration of sodium chloride (Cañedo-Argüelles et al., 2017). This drainage may be reduced using natural processes, such as evapotranspiration (Rauche, 2015). Evapotranspiration is the second major component in the water cycle, after precipitation (Lamb, 2015). Researchers have estimated that 60% of continental precipitation is transported to the atmosphere by evapotranspiration (Novák, 2012). Evapotranspiration is the sum of evaporation of water from soil and transpiration from plants (Lamb, 2015). Evapotranspiration is important as it consumes energy (Novák, 2012), regulates the temperature of leaves and soil (Thornthwaite, 1948), determines the water requirements for crops and irrigation schedules (Goyal and Harmsen, 2014), and recharges surface and ground water (Tukimat et al., 2012). Additionally, the selection of crops and production regions are also based on evapotranspiration studies (Goyal and Harmsen, 2014).

Evapotranspiration rates are governed by weather conditions, such as solar radiation, temperature, wind

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speed, water vapor concentration gradients (Allen et al., 1998), available moisture at the root zone, land management (Thornthwaite, 1948), plant type and growth stage (Doorenbos and Pruitt, 1977). Three main concepts describe evapotranspiration: reference evapotranspiration, crop evapotranspiration and actual evapotranspiration (Goyal and Harmsen, 2014; Allen et al., 1998). Reference evapotranspiration (ET_o) refers to water consumption by a hypothetical grass, with uniform height (0.12 m) and not limited by water or nutrients (Allen et al., 1998). Crop evapotranspiration (ET_c) incorporates evaporation and transpiration by a field crop under optimal conditions (Allen et al., 1998), whereas actual evapotranspiration (ET_a) indicates the quantity of water removed from crops under nonstandard environments (Allen et al., 1998).

Actual evapotranspiration can be measured using lysimeters (Goyal and Harmsen, 2014). Lysimeters evaluate evapotranspiration by measuring water balance components, e.g., precipitation, surface runoff, drainage and variation in soil-water storage (Abtew and Melesse, 2013). Nevertheless, lysimeter measurements represent a specific area and have high operation and maintenance costs (Abtew and Melesse, 2013). Hence, observational data should be used to calibrate evapotranspiration models allowing one to make predictions (Goyal and Harmsen, 2014; Radcliffe and Šimůnek, 2010).

Several studies have simulated water flow processes using Hydrus code (Kodešová et al., 2014; Li et al., 2014). Hydrus is one of the most robust models for simulating water flow in up to three dimensions (Šimůnek et al., 2008). Hydrus simulates infiltration, evaporation, transpiration, redistribution, and discharge water through saturated and unsaturated media using the Richards equation (Šimůnek et al., 2008; Radcliffe and Šimůnek, 2010). Heat and solute flows within the media can also be studied via advection-dispersion equations (Radcliffe and Šimůnek, 2010; Lamb, 2015).

However, few studies have been conducted to simulate water fluxes from evapotranspiration covers for potash tailings piles using experimental field data, because it is expensive to conduct lysimeter experiments on potash tailings piles; the steep slopes of the piles, 40^o, make it difficult to install experiments; and the saline nature of the potash tailings piles, containing approximately 90% salt, prevent crop growth. Evapotranspiration covers, also known as water balance covers, soil-plant covers or store-and-release covers (Rock et al., 2012), use a precipitation soil reservoir and a vegetation cover to move the moisture back to the atmosphere (Hauser, 2009). Regarding the soil, Hauser (2009) suggests the use of local materials to reduce transport costs. The soil should have a high water retention capacity and fertility to guarantee the vegetation’s growth (Hauser, 2009). Evapotranspiration covers are used to reduce the water infiltration into waste systems, decrease the seepage from the wastes to ground water, control emission of gases (Hauser et al., 2001), decrease erosion and exposure to the wastes and restore the landscape (Rock et al., 2012; Hauser, 2009). The performance of evapotranspiration covers is generally evaluated by measuring or estimating the seepage (Rock et al., 2012). This is achieved by determining all water balance components (Hauser et al., 2005). Estimating evapotranspiration is important because it is the largest output term and controls the size of the other water balance components (Hauser et al., 2005).

Therefore, the aim of this study was to calibrate and test the Hydrus-1D to make predictions using observational data from a lysimeter experiment. More specifically, this study aims to evaluate the meteorological conditions of the experimental site, drainage and evapotranspiration from substrates, composed of municipal solid waste incineration bottom ashes and coal combustion residues. This research additionally examines the water fluxes in Hydrus-1D using daily precipitation, air temperature, solar radiation, wind speed and relative air humidity from a weather station located approximately 20 km away. Last, this article aims to predict evapotranspiration and drainage by using different values of fine fraction, soil texture and crop parameters, such as root depth and crop height.

2 Material and methods

2.1 Experimental site and design

The experiment was conducted on the potash tailings pile at the Wintershall potash plant, 50° 53' 160" north and 9° 59' 12" east, on the outskirts of Heringen, Germany. The experiment included 4 treatments with two repetitions, using eight nonweighable lysimeters. The lysimeters were 3 m deep and each covered an area of 2 m². The treatments comprised four substrates made of different proportions of municipal solid waste incineration bottom ashes (12-mm sieve) and coal combustion residues.

Substrate 1 was composed of 80% municipal solid waste incineration bottom ash and 20% coal combustion residues. Substrate 2 was composed of 70% municipal solid waste incineration bottom ash and 30% coal combustion residues. Substrate 3 was composed of 60% municipal solid waste incineration bottom ash, 10% washed sand from gravel extraction, and 30% coal combustion residues. Substrate 4 was composed of 50% municipal solid waste incineration bottom ash, 30% coal combustion residues, 10% furnace bottom ash with particle sizes between 0.2 and 2 mm, and 10% of the original bottom ash with particle sizes from 0 to 6.3 mm (Schmeisky and Papke, 2013).

A seed mixture containing 65% perennial ryegrass (*Lolium perenne* L.), 25% red fescue (*Festuca rubra* L.) and 10% Kentucky bluegrass (*Poa pratensis* L.) was sowed from 5 August to 26 September 2013, totaling 70 g m^{-2} (Schmeisky and Papke, 2013). In addition, the annual quantity of fertilizer applied was 83 g m^{-2} in 2013, 193 g m^{-2} in 2014, 94 g m^{-2} in 2015, and 158 g m^{-2} in 2016, consisting of 61 g m^{-2} of nitrogen, 80 g m^{-2} of phosphorus, 79 g m^{-2} of potassium and 9 g m^{-2} of magnesium (Schmeisky and Papke, 2013; Papke and Schmeisky, 2017).

2.2 Meteorological data

Micrometeorological parameters were registered automatically by a Thies-Clima weather station, equipped with a Datalogger DLx-MET. Wind speed (m s^{-1}, 3-m height), air temperature (2-m height), soil temperature (0.3-m depth), relative air humidity (2-m height) and solar radiation (2-m height) were recorded at 10-min intervals. Precipitation was assessed by the Thies weather station using a tipping bucket system, in addition to 4 rain gauges installed at ground level and 5 gauges installed at 1-meter height (Table 1).

Table 1 Meteorological data from the Heringen experimental field site during three hydrological years

Parameter	Unity	2014	2015	2016	Mean	±	CV
Precipitation ground-level gauges (Σ)	mm	788.3	543.8	683.9	672.0	122.7	18.3
Precipitation Thies weather station (Σ)	mm	778.8	508.1	-	-	-	-
Precipitation 1-m high gauges(Σ)	mm	710.0	484.9	603.4	599.4	112.6	18.8
Minimum air temperature (Ø)	°C	6.8	5.8	6.7	6.4	0.6	8.6
Maximum air temperature (Ø)	°C	13.8	13.0	13.7	13.5	0.4	3.2
Mean air temperature (Ø)	°C	10.0	9.2	10.0	9.7	0.5	4.7
Mean substrate temperature (Ø)	°C	11.0	10.2	10.7	10.6	0.4	3.8
Relative air humidity (Ø)	%	82.4	80.0	81.6	81.3	1.2	1.5
Wind speed / 2-m height (Ø)	m s^{-1}	2.5	2.9	2.7	2.7	0.2	7.4
Solar radiation (Ø)	W m^{-1}	118.9	127.0	122.9	122.9	4.1	3.3
$ET_{(H)}$ (Σ)	mm	508.9	571.7	503.2	527.9	38.0	7.2
ET_o-n/ref (Σ daily)	mm	647.5	721.4	675.8	681.6	37.3	5.5
ETc (Σ)	mm	670.8	750.9	703.1	708.3	40.3	5.7

Note: Ø is the average value, Σ is the sum value, $ET_{(H)}$ is Haude´s potential evapotranspiration, ET_o is the reference evapotranspiration, ET_c is the crop evapotranspiration, ± refers to the standard deviation, CV is the coefficient of variation

Table 2 Water retention curve parameters according to Van Genuchten (1980) model of the substrate 1

Depth m	B_d g cm^{-3}	θ_r	θ_s	α 1 cm^{-1}	m	n	R^2	K_s cm d^{-1}
		----- cm^3 cm^{-3} -----						
0.0-0.04	1.16	0.000	0.5202	0.0728	0.1794	1.2186	0.9937	785.5
0.20-0.24	1.17	0.000	0.5160	0.1082	0.1654	1.1982	0.9926	902.7
0.40-0.44	1.25	0.000	0.4860	0.0745	0.1748	1.2118	0.9935	546.9
0.60-0.64	1.23	0.000	0.4909	0.0636	0.1765	1.2144	0.9913	514.5
Mean	1.20	0.000	0.5038	0.0777	0.1737	1.2103	0.9933	687.4

Note: B_d is the bulk density; θ_r is the residual water content; θ_s is the saturation water content; α, m, n are empirical shape parameters; R² (R squared) is the coefficient of determination; K_s is the saturated hydraulic conductivity

2.3 Drainage and evapotranspiration assessment

The drainage from the lysimeters was collected using discharge lines, and the actual evapotranspiration was determined using the simplified water balance expression:

$$ET_a = P - D \quad (1)$$

Where ET_a is the actual evapotranspiration (mm), P is the ground-level precipitation (mm), and D is the lysimeters' drainage (mm).

2.4 Simulations and calibration of Hydrus-1D

The forward simulation of the water fluxes from substrates 1-4 was performed with the experimental observations from 2014 to 2015. The hydrological year 2016 was not considered due to the lack of precipitation data from the Thies weather station (Table 1). Four materials were used to simulate water flow within the lysimeters, because 4 sets of hydraulic properties per substrate were measured (Table 2).

The potential evapotranspiration was estimated using the Penman-Monteith equation according to the formulation of Šimůnek et al. (2013), using the meteorological parameters measured by the Thies weather station. Moreover, the potential evapotranspiration considered a root depth of 0.10 m in October 2014 and 0.18 m in October 2015 (Papke and Schmeisky, 2017). The crop height was set to 0.30 m during the two hydrological years. Leaf area index was estimated in Hydrus-1D from the crop height of alfalfa and other field crops, since it is recommended in the Hydrus-1D manual for crop height to be between 0.10-0.50 m (Šimůnek et al., 2013).

The Feddes root uptake reduction model for grasses was used to simulate the actual root water uptake (Radcliffe and Šimůnek, 2010). The relative root distribution was distributed linearly from 1 at the substrate surface (0.01 m depth) to zero at the lower profile of the root depth (0.18 m depth). Initial pressure head increased linearly from -100 hPa at the substrate surface to zero at the bottom of the substrates. This initial pressure was set because the general field capacity of coarse soils is -100 hPa (Radcliffe and Šimůnek, 2010). Observed points were placed at 0.05, 0.10, 0.20, 0.40, 0.60, 1.20, 2.00, 2.40 and 2.60 m depth, where drainage occurs (Figure 1).

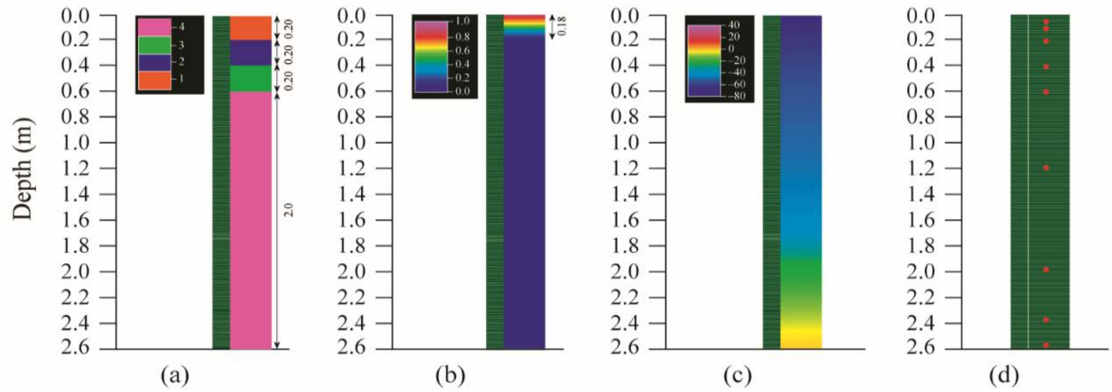


Figure 1 (a) Material distribution; (b) root distribution; (c) initial pressure head; (d) observation points for the forward simulation using Hydrus-1D

Table 3 Inverse solution data for the Hydrus 1-D calibration

Parameters	Drainage		Water content		ψ_m[1](Θ)		Total number (N) of
	Nr.	Weight	Nr.	Weight	Nr.	Weight	observations
Inverse 1	104	1	1	1	0	-	105
Inverse 2	4	1	1	1	0	-	5
Inverse 3	-	-	19	1	1	10	20
Inverse 4	4	10	19	1	0	-	23
Inverse 5	24	10	19	1	0	-	43

Note: [1] ψ_m at 30 hPa

The atmospheric boundary was selected as the upper boundary condition, and the seepage face as the lower boundary condition. For Hydrus-1D calibration by the inverse solution, five different input data were used to optimize the hydraulic parameters of the substrates (Šimůnek et al., 2008). Moreover, following the recommendation of Rassam et al. (2003), more than one data set was used to calibrate the Hydrus-1D (Table 3).

The first calibration was performed using 104 weekly observations of the drainage and 1 water content measurement, evaluated on 25.06.2015 from 0.0 – 0.06 m depth. The second optimization was made using 1 water content measurement and the seasonal cumulated drainage of the substrates (winter and summer 2014, winter and summer 2015). The third calibration considered 19 weekly observed water content (from 25.06.2015 to 29.10.2015), and one retention curve measurement, $\psi_m(\Theta)$, weight 10. The fourth included 19 water content measurements and 4 seasonal cumulated drainage measurements, weight 10. The fifth calibration type consisted of using 24 monthly observations of the drainage (weight 10), and 19 weekly measurements of water content. The weight for each measurement represents the importance of the data for the calibration (Radcliffe and Šimůnek, 2010).

Different arrangements of fixed and optimized Van Genuchten hydraulic parameters were evaluated; however, the Hydrus-1D converged for all substrates when the volumetric water content at saturation (θ_s), the saturated hydraulic conductivity (K_s) and the fitted parameters of the water retention curve (n, α) were optimized. The residual water content (θ_r), was fixed to 0.001 $cm^3\ cm^{-3}$, and the pore connectivity to 0.5. After running the calibration, the coefficient of determination (R-squared) was observed, as well as the mass balance error, iteration number and calculation time, root-mean-square error (RMSE), and absolute differences between measured and estimated values of drainage, actual evapotranspiration and water content of the substrates.

The coefficient of determination, R-squared, shows how well the optimized model replicates the observed values (Šimůnek et al., 2013). Mass balance error (%) is the relative error of the water balance fluxes. The number of iterations represents the number of solutions of the global matrix equations to converge the model (Šimůnek et al., 2013). The root-mean-square error (RMSE) estimates the differences between observed and predicted values (Schaap et al., 2001).

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(O_i - P_i)^2} \quad (2)$$

Where O and P are the observed and predicted values, referring to the cumulated seepage (mm) or water content ($cm^3\ cm^{-3}$); and N is the number of observations.

The calibrated Hydrus-1D that exhibited the best agreement with the observed values was then used to simulate the water fluxes for tested substrates over 27 hydrological years, from 1 November 1989 to 31 October 2016 using daily weather data from Bad Hersfeld (Deutsche Wetterdienst, 2017).

2.5 Evapotranspiration and drainage under differing fine fractions and soil textures

Water fluxes were studied using 60%, 80% and 100% fine fractions (particles < 2 mm). For this, the field disturbed samples of the substrates from 0.40 to 0.64 m depth were air dried in the laboratory for approximately 10 days. Then the substrates were sieved to obtain fine, < 2 mm of diameter, and coarse fractions, > 2 mm of diameter. In this sequence, 100 g of substrates were packed in stainless cylinders according to the different fine fractions based on the oven dried weight. After shaking the cylinders 100 times to settle the substrates, the height covered by the substrates was measured and the substrate´s volume was estimated. Later the samples were saturated for 48 h and oven dried at 105°C up to a constant weight. Three repetitions were performed, resulting in 36 samples. With the determined bulk densities and the particle size distribution previously estimated with the disturbed samples from the field, the hydraulic parameters of the substrates were found using the Rosetta pedotransfer function (Radcliffe and Šimůnek, 2010; Schaap et al., 2001), which is implemented in the Hydrus-1D Software, version 4.16.0110 (Šimůnek et al., 2014; Rassam et al., 2003). The Rosetta-based pedo-transfer function was also used to determine the hydraulic parameters of different soil textures, such as clay loam, silt loam and sandy loam soils.

Further simulations were conducted following the approach suggested by Brakensiek et al. (1986), who state that the saturated hydraulic conductivity decreases according to the relative stone content (stoniness).

$$K_r = \frac{K_{se}}{K_s} = 1 - R_w \quad (3)$$

Where K_r is the relative hydraulic conductivity, K_{se} is the effective saturated hydraulic conductivity of stony soils (cm d^{-1}), K_s is the saturated hydraulic conductivity of fine earth (cm d^{-1}), and R_w is the relative stone content in mass units. In contrast, the fitted parameters of the Van Genuchten model, i.e., α, m and n, are assumed to be constant (Beckers et al., 2016).

2.6 Statistical analysis

An evaluation of the meteorological data and water balance components was conducted for three hydrological years, 2014, 2015 and 2016. Descriptive statistics were used to summarize the data set from the measurements. The central tendency of the data was determined using mean values, whereas the variability of the mean was determined as standard deviation and the coefficient of variation.

Correlation studies were conducted using the Spearman and Pearson correlation coefficients, based on the Shapiro-Wilk normality test (Field, 2013). The correlation and normality tests were performed using RStudio, version 0.99.491 (RStudio Team, 2015).

3 Results and discussions

3.1 Observed substrate water fluxes

The actual evapotranspiration and the drainage of the different substrates during 2014, 2015 and 2016 are shown in Figure 2. The mean drainage of substrates 1-4 was 271.2 mm in 2014, 192.1 mm in 2015 and 231.1 mm in 2016. A low coefficient of variation among the substrates was observed for drainage, which was 3.6% in 2014, 6.4% in 2015 and 5.5% in 2016. The ratio between drainage and ground-level precipitation (D/P) averaged 34.4% in 2014, 35.3% in 2015 and 33.8% in 2016.

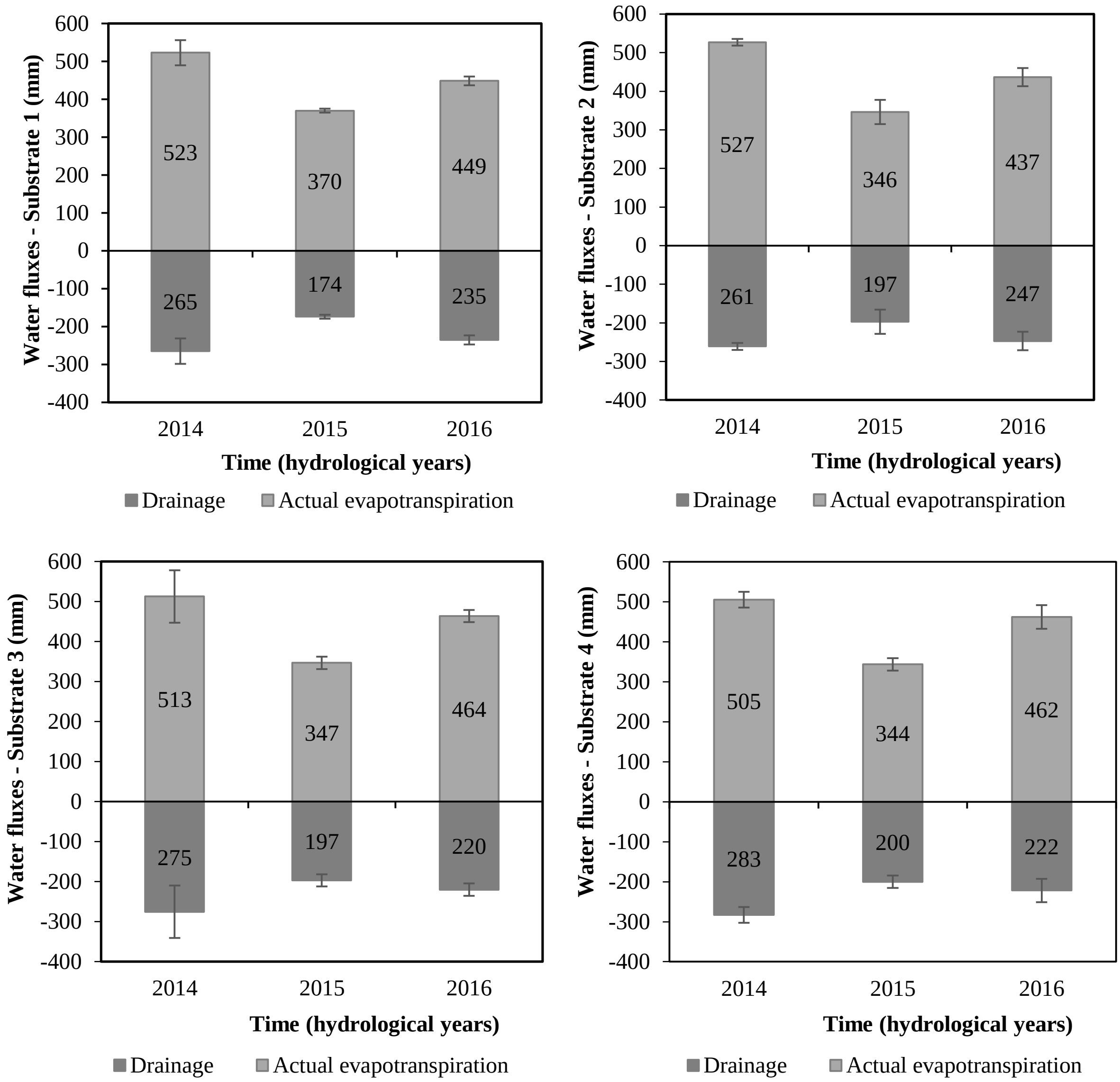


Figure 2 Observed water fluxes of substrates 1-4 during 2014, 2015 and 2016 (± standard deviation)

Following the trend of the drainage, the actual evapotranspiration was 517.1 mm in 2014, 351.7 mm in 2015 and 452.8 mm in 2016. The actual evapotranspiration registered low variation among the substrates in 2014 (1.9%), 2015 (3.5%) and 2016 (2.8%). The ratio between actual evapotranspiration and precipitation averaged 65.6% in 2014, 64.7% in 2015 and 66.2% in 2016. These results were discussed by Bilibio et al. (2017), Bilibio (2018) and Bilibio et al. (2021). Care must be taken to extrapolate the results of the actual evapotranspiration because the water storage change was not considered in the simplified water balance equation (Equation 1).

3.2 Forward simulation, calibration and examination of the Hydrus-1D

Forward simulation of water fluxes was performed with Hydrus-1D, using hydraulic properties from the substrates and weather data from 2014-2015. The simulations revealed a high coefficient of determination (R^2) for the observed drainage and moderate coefficient of determination for the water content values (Table 4). However, the absolute differences between measured and predicted drainage were found to be high. For instance, substrate 1 registered 23.0 mm less than the total observed drainage; substrate 2, -93.7 mm; substrate 3, -94.3 mm; and substrate 4, -90.5 mm, comprising a mean variation of -16%. The highest RMSE (52.2 mm) was found for substrate 3, and the lowest (34.8 mm) for substrate 1 (Table 4).

Table 4 Root-mean-square error (RMSE) and correlation coefficients between observed and forward simulations of drainage and water content using Hydrus-1D with substrates 1-4

Substrates	Drainage RMSE mm	Drainage Correlation coefficient	Drainage Correlation *p*-value	Drainage R^2	Water content RMSE $cm^3\ cm^{-3}$	Water content Correlation coefficient	Water content Correlation *p*-value	Water content R^2
Substrate 1	34.8	0.99	<0.001	0.98	0.063	0.80	<0.001	0.64
Substrate 2	49.9	1.0	<0.001	1.0	0.086	0.71	<0.001	0.50
Substrate 3	52.2	0.98	<0.001	0.96	0.064	0.74	<0.001	0.55
Substrate 4	49.4	1.0	<0.001	1.0	0.068	0.73	<0.001	0.53

Considering these results, the Hydrus-1D was calibrated according to different inverse solution data (Table 3). A high association between calibrated and measured values ($R^2 > 0.9$) was observed for all calibration methods, except when using the water content and retention curve measurements ($0.8 \le R^2 \le 0.92$). Further analyses revealed the number of iterations were within the initial configuration of the Hydrus-1D, up to 20 iterations. The calculation time of the inverse solution ranged from 19 to 53.9 seconds, which is considered low. In addition, the water mass balance errors were lower than 1%, which is the upper limit for water balance assessments (Radcliffe and Šimůnek, 2010).

The highest estimate of root-mean-square error (RMSE) was registered for the calibration using water content and retention curve values (inverse solution 3), with 75.9 mm for substrate 1, 163.1 mm for substrate 2, 51.5 mm for substrate 3, and 35.1 mm for substrate 4. When the drainage observations were used in the inverse simulation, the RMSE was similar among the models. However, the inverse simulation using 104 measurements of drainage and one reading of water content exhibited the lowest RMSE for water content, with 0.065 $cm^3\ cm^{-3}$ in substrate 1, 0.058 $cm^3\ cm^{-3}$ in substrate 2, 0.079 $cm^3\ cm^{-3}$ in substrate 3, and 0.091 $cm^3\ cm^{-3}$ in substrate 4.

The absolute differences between predicted and observed values of the cumulated drainage and actual evapotranspiration were also examined. The highest differences were observed when using water content and retention curve measurements (calibration type number 3, Table 3). Lower differences between predicted and observed drainage were estimated when the inverse simulation was performed using drainage measurements. For instance, by using 104 drainage measurements in the Hydrus inverse solution, the differences between observed and predicted values ranged from -1.3% in substrate 1 to -5.1% in substrate 4 (mean -2.9%, -13.6 mm). Nevertheless, the inverse simulations using 104 drainage measurements predicted higher total actual evapotranspiration, approximately 7.3% (63.3 mm), than in the observed measurements. These differences can be related to salt stress (Šimůnek et al., 2013), nutrient availability (Blume et al., 2016) or any change in the grass cover in the field (Allen et al., 1998), i.e., natural integration of native crops (Papke and Schmeisky, 2013).

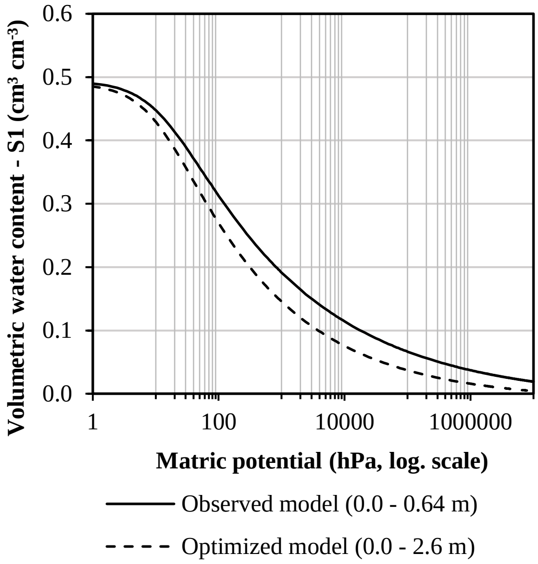
While assessing the hydraulic parameters of the substrates, the inverse simulation increased the values of the fitted parameters from the Van Genuchten (1980) model, α and n, causing the water retention curves to shift to the left. This means that for the same matric potential, the substrates retain less moisture. Figure 3a shows examples for substrate 1. Substrates 2-4 showed a similar trend. These differences between observed and optimized fitted parameters of the water retention curve may be related to the use of fine fractions on the edges of the cylinders in the field to improve contact with the suction ceramic plates in the laboratory. An increasing trend of the fitted parameters of the water retention curve is expected when using coarser materials (Rassam et al., 2003; Schaap et al., 2001). Moreover, the differences in size of the flow domain (cylinder samples and 2.6 m depth lysimeters) and the wetting and drying processes in the field – hysteresis (Hopmans, 2010) – can also contribute to differences between measured and optimized fitted parameters of the water retention curve (Kodešová et al., 2014).

For saturated hydraulic conductivity, the inverse simulations provided lower values than the ones measured in the laboratory. For example, the mean saturated hydraulic conductivity of substrate 1 from 0.0 to 0.64 m depth was 687.4 cm d^{-1}, whereas the optimized parameter was 182.14 cm d^{-1}. This may be due to errors in the laboratory measurements, such as water flow in the internal walls of the cylinders, and sample size (Shukla, 2014).

Considering the differences between observed and predicted drainage, actual evapotranspiration and water content, the inverse simulation conducted with 104 observations of drainage and one measurement of water content was used to carry out further studies.

Figure 3b shows the observed versus predicted cumulated drainage values from substrate 1 using the mentioned inverse simulation. Differences between predicted and observed drainage can be attributed to macropores, cracks and lateral flow on the lysimeter walls (Li et al., 2014), which are not considered in the Richards equation (Van Genuchten, 1992).

(a)



(b)

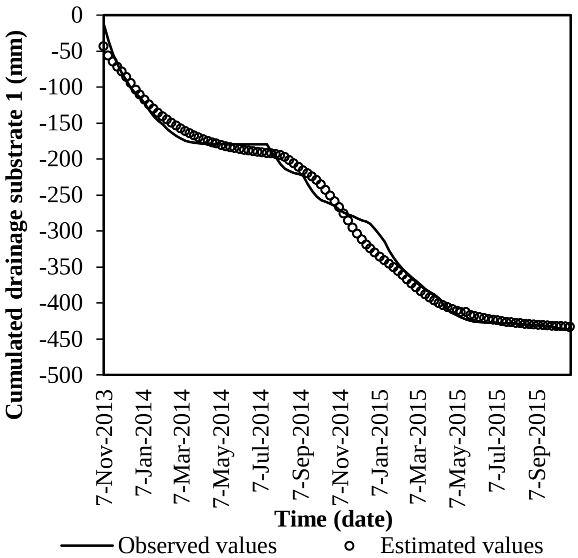


Figure 3 (a) Observed and optimized water retention curve from substrate 1. (b) Observed versus predicted cumulative drainage of substrate 1 using 104 observations of drainage and one measurement of water content in the inverse solution of Hydrus-1D during two hydrological years

Note: The solid line is the observed model from 0.0 to 0.64 m depth, and the dashed line is the optimized model from 0.0 to 2.60 m depth in (a). The solid line is the observed drainage and the dashed line is the predicted cumulative drainage in (b).

Figure 4 shows the cumulative and daily potential and actual root water uptake from substrate 1, whereas Figure 5 highlights the predicted daily water content in substrate 1 at different observation points. Substrates 2-4 showed similar values. Figure 6 illustrates the water storage change of substrates 1-4 in the entire flow domains of the lysimeters from 0.0 to 2.6 m depth.

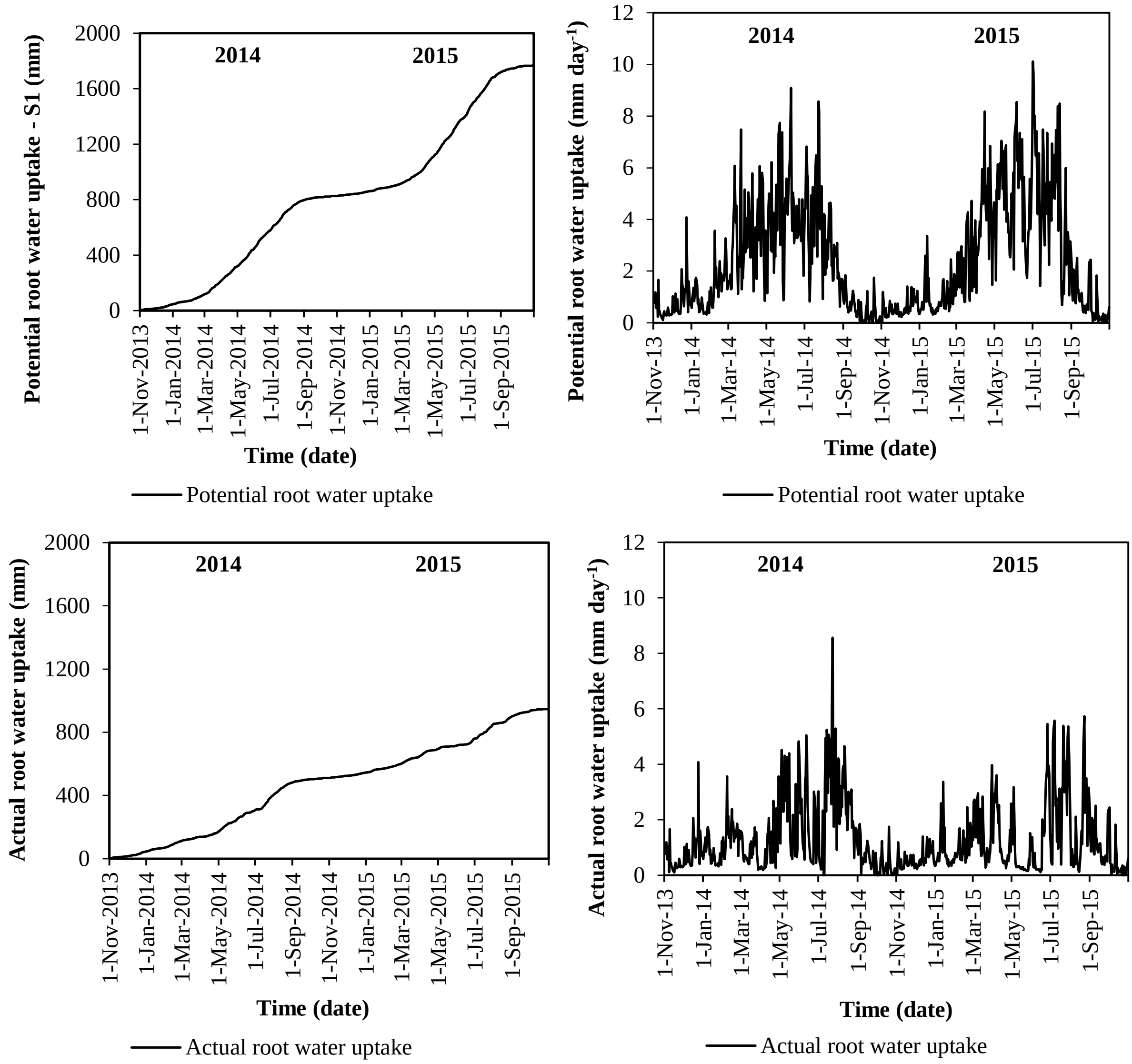


Figure 4 Predicted potential and actual root water uptake (cumulative - mm, and daily values – mm day^{-1}) of substrate 1 using 104 observations of drainage and one measurement of water content in the inverse solution of Hydrus-1D over two hydrological years

The cumulative and daily actual root water uptake (means for S1-S4: 932.4 mm, 1.3 mm d-1) of the substrates were generally lower than the potential root water uptake (means for S1-S4: 1766.7 mm, 2.4 mm d-1), Figure 4. This is because the potential root water uptake considers no limitation of water or nutrients (Allen et al., 1998). Additionally, higher daily values of potential root water uptake and actual root water uptake were observed in summer months (from May to October), which registered higher radiation and temperature levels. The mean potential root water uptake in the summer was 3.14 mm d-1, and the actual root water uptake was 1.58 mm d-1. On the other hand, in winter (from November to April) the mean potential root water uptake was 1.69 mm d-1, and the actual root water uptake was 0.95 mm d-1 for substrates 1-4.

The predicted daily water content levels at different observation points (Figure 5) show that the water content oscillates at 0.6 m depth and above. In deeper layers, the water content is more constant. The substrate surface is more exposed to meteorological conditions, such as precipitation, wind and temperature (Kodešová et al., 2014). In addition, root water uptake takes place near the surface, which contributes to the variability of the water status in this region (Radcliffe and Šimůnek, 2010; Lal and Shukla, 2004).

From the predicted daily water storage of substrates 1-4, Figure 6, it is possible to observe that water storage in the substrates increases in winter and decreases in summer, following the pattern of root water uptake. The greater increase in water storage in July 2014 may be due to the rain cumulated during this month. Ground-level gauges registered 237.6 mm and the Thies weather station 221.6 mm in July 2014. During this period, the stored water increased 113.2 mm in substrate 1, 110.7 mm in substrate 2, 115.2 mm in substrate 3 and 117.0 mm in substrate 4.

Water storage capacity values of the substrates expressed through the field capacity, i.e., hydraulic conductivity close to 0.01 cm d-1 (Šimůnek et al., 2014), at 2.6 m depth, were: 721.8 mm for substrate 1 (277.6 mm m-1); 647.73 mm for substrate 2 (249.1 mm m-1); 589.1 mm for substrate 3 (226.6 mm m-1); and 555.7 mm for substrate 4 (213.7 mm m-1) according to the calibrated Hydrus-1D. In evapotranspiration covers the water storage capacity represents the rain moisture that can be stored in the substrate layer (Hauser, 2009). Part of this moisture is subsequently transported by the vegetation cover to the atmosphere (Hauser, 2009).

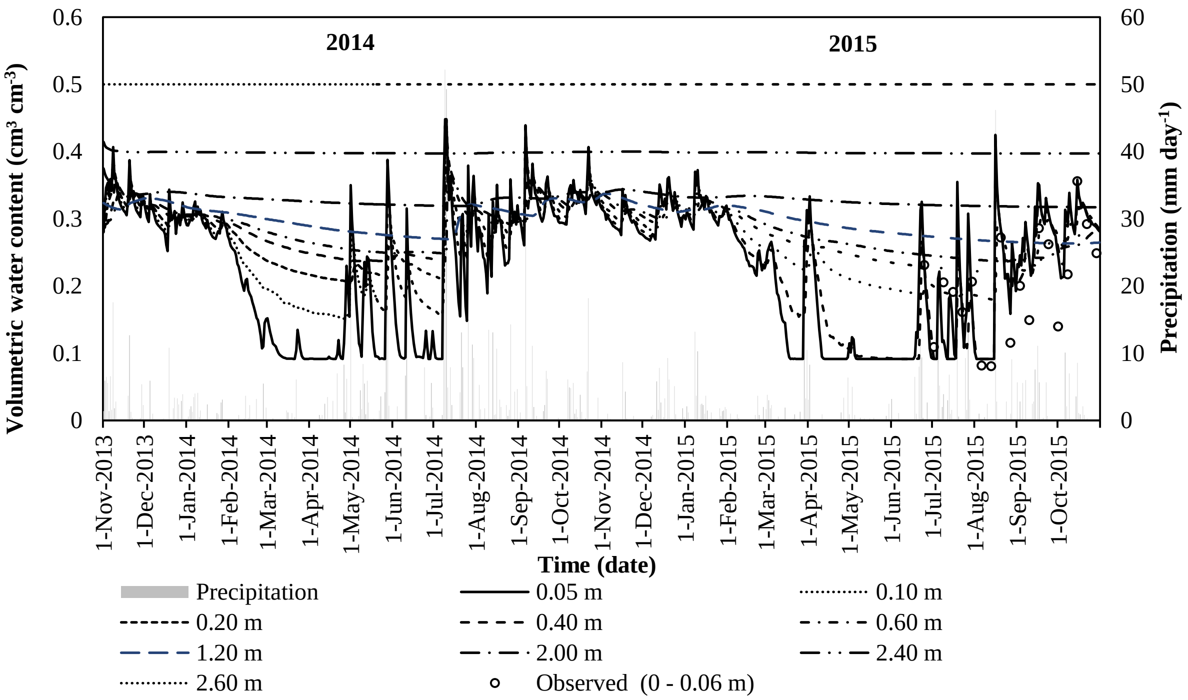


Figure 5 Predicted water content levels at different observation points for substrate 1 using 104 observations of drainage and one measurement of water content in the inverse solution of Hydrus-1D during two hydrological years

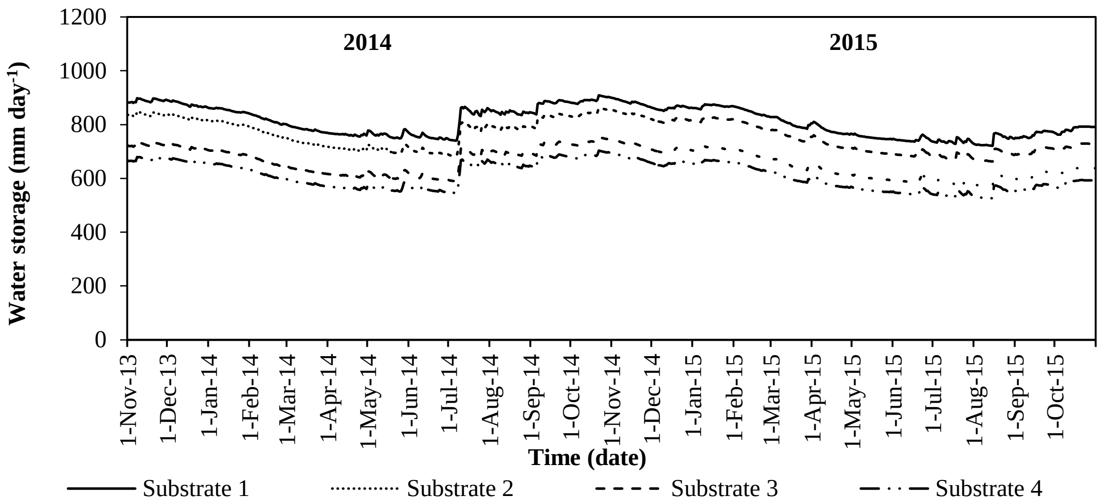


Figure 6 Predicted water storage of substrates 1-4 in the entire flow domains of the lysimeters, from 0.0 to 2.6 m depth

3.3 Examination of the calibrated Hydrus-1D and predictions

Due to the lack of precipitation measurements from the Thies weather station in 2016, the daily weather data available for Bad Hersfeld was used to examine the calibrated Hydrus-1D. Twenty-seven hydrological years, from 1990 to 2016, were studied. For this simulation, a constant root depth of 0.18 m and a crop height of 0.30 m were used. An cumulated precipitation of 1809.9 cm (mean 67 cm yr^{-1}) was observed. The potential root water uptake was 2004.3 cm (mean 74.2 cm yr^{-1}), actual root water uptake 1360.8 cm (mean 50.4 cm yr^{-1}, and cumulated drainage 429.4 cm (mean 15.9 cm yr^{-1}). Moreover, the total evaporation was 14.9 cm over 27 years (mean 0.6 cm yr^{-1}). Considering the ratio between drainage and precipitation (D/P), a drainage rate of 23.7% was estimated using the hydraulic parameters of substrate 1, 23.7% for substrate 2; 25.3% for substrate 3; and 26.1% for substrate 4. These results agree with those of Hermsmeyer (2001), who found a drainage rate of 24.4% from a technogenic substrate made of aluminum recycling by-products (70%) and flue gas desulfurization by-product (30%), covering a potash tailings pile located near Hannover, Germany. However, if the crop height is decreased from 0.30 to 0.20 m, a mean drainage rate of 27.3% is obtained. In addition, if the root depth is increased to 0.28 m, and crop height maintained at 0.30 m, the calibrated Hydrus-1D predicts a mean drainage rate of 22.2%, which is slightly lower than the inverse simulations using a root depth of 0.18 m (mean of S1-S4: 24.7%). This shows that the water fluxes of the evapotranspiration covers are affected by any change in crop status. The crop height is used to estimate leaf area index, crop canopy and aerodynamic resistances in the Penman-Monteith equation (Šimůnek et al., 2013). The root depth represents the substrate area explored by the roots, from which water is transported to the atmosphere (Radcliffe and Šimůnek, 2010). However, long-term predictions in the future should consider effects of structure formation, pore changes and biopore development (Blume et al., 2016) on the substrates. The values for drainage for different root depths and crop heights for 27 water-years for Bad Hersfeld using optimized hydraulic parameters from substrate 1 are shown in Figure 7.

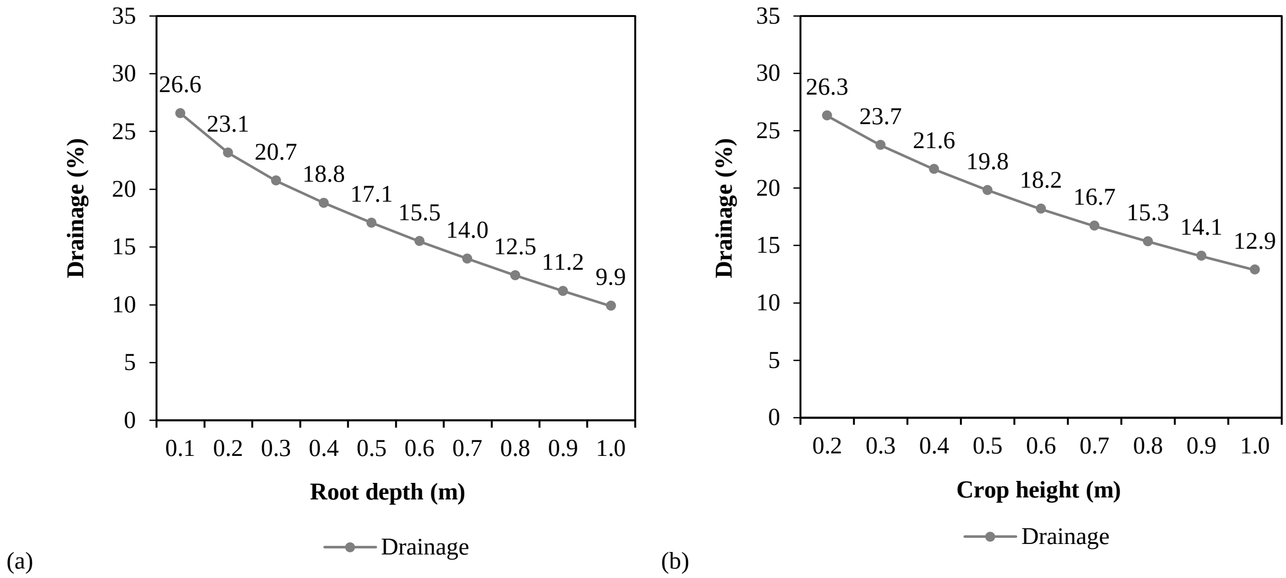


Figure 7: Drainage precipitation ratio for different root depths (a) and crop heights (b) for 27 hydrological years for Bad Hersfeld, using optimized hydraulic parameters from substrate 1

Examining the hydrological years more closely, one observes a variation of approximately 38.9% for drainage and 20.5% for actual evapotranspiration. This variation is higher than values observed during the three hydrological years in Heringen, 17.1% for drainage and 18.9% for actual evapotranspiration among the hydrological years from 2014 to 2016 (Figure 2). However, this may be expected due to the variation in precipitation, solar radiation, temperature and cloudiness during the growing season of the perennial grasses.

3.4 Water fluxes considering different fine fractions and soil textures

The water fluxes were simulated using 60%, 80% and 100% fine particles. For the drainage, a cumulative predicted drainage rate of 332.7 mm was observed using 60% fine particles, 291.0 mm using 80% fine particles, and 259.6 mm using 100% fine particles in Heringen from 2014 to 2015. A similar pattern was found for the simulated water fluxes using different soil textures. Clay loam registered the lowest total drainage (391.9 mm), whereas the highest (520.4 mm) was found using sandy loam (Table 5).

Table 5 Mean hydraulic parameters and cumulated drainage using 60%, 80% and 100% fine fraction of substrates 1-4 and soil textures from 2014 to 2015 in Heringen

Fine earth	θ_r	θ_s	α	n	K_s	Volume[1]	Total drainage		Differences	
	$cm^3\ cm^{-3}$	$cm^3\ cm^{-3}$	$1\ cm^{-1}$		$cm\ d^{-1}$	mm	mm	%	mm	%
100%	0.0373	0.4066	0.0115	1.5014	101.2	459.6	259.6	20.2		
80%	0.0362	0.3934	0.0126	1.4923	81.3	458.3	291.0	22.6	31.5	12.1
60%	0.0352	0.3820	0.0141	1.4815	65.7	459.5	332.7	25.9	73.1	28.2
Clay loam	0.095	0.41	0.019	1.31	6.24	768.3	391.9	30.5		
Silt loam	0.067	0.45	0.02	1.41	10.8	708.5	421.8	32.8	29.9	7.6
Sandy loam	0.065	0.41	0.075	1.89	106.1	362.7	520.4	40.4	128.5	32.8

Note: Soil water storage at field capacity in 2.6 m deep

When applying the approach of relative stone content for the water retention curve parameters (Beckers et al., 2016) of the calibrated Hydrus-1D from substrate 1, a decreasing trend of 7.8% was found for drainage when increasing the percentage of fine fraction from 60% to 80%, in Bad Hersfeld over 27 years of historical weather data (Table 6).

Table 6 Cumulated drainage using the relative stone content approach for substrate 1 from 1990 to 2016 in Bad Hersfeld

Fine earth	θ_r	θ_s	α	n	K_s	Volume[1]	Total drainage		Differences	
	$cm^3\ cm^{-3}$	$cm^3\ cm^{-3}$	$1\ cm^{-1}$		$cm\ d^{-1}$	cm	cm	%	mm	%
80%	0.0	0.600	0.0893	1.2597	218.6	85.68	396.1	22.0	-33.3	-7.8
60%[2]	0.0	0.500	0.0893	1.2597	182.1	72.18	429.4	23.8	-	-
40%	0.0	0.400	0.0893	1.2597	145.7	58.47	470.6	26.1	41.2	9.6
Clay loam	0.095	0.41	0.019	1.31	6.24	76.83	442.9	24.6	-	-
Silt loam	0.067	0.45	0.02	1.41	10.8	70.85	398.5	22.1	-44.4	-10.0
Loam	0.078	0.43	0.036	1.56	24.96	57.42	479.9	26.6	37.0	8.4

Note: Soil water storage at field capacity in 2.6 m deep. [2] Substrate 1 - calibrated model

The various approaches used to study the use of fine fractions, including bulk densities, soil textures and relative stone content, indicated that lower drainage rates of evapotranspiration covers may be obtained by increasing either the proportion of fine particles (< 2 mm) or the clay and silt size particles in the technogenic substrates. Root development, i.e., root length and root depth, is also expected to improve by increasing the fine fraction (Babalola and Lal, 1977) and lead to further reduction in drainage. Fine particles can additionally be used as interlayers in evapotranspiration covers, as is recommended in capillary barriers (Radcliffe and Šimůnek, 2010).

4 Conclusions

The present study calibrated the Hydrus-1D to make predictions about evapotranspiration and drainage from potash tailings covers. The observed hydraulic properties, drainage and water content of four different technogenic substrates provided the inputs to optimize the Van Genuchten water retention parameters.

The inverse simulation using weekly measurements of the drainage provided lower differences between predicted and measured drainage and water content values. The calibrated Hydrus-1D showed a mean variation between the observed and predicted values of 2.9% (approximately 13.6 mm) for the cumulated drainage of substrates 1-4 from 2014 to 2015, which is lower than the direct simulation (approximately 16% or 75.4 mm).

The inverse simulation using surface water content and water retention curve measurements deviated from the observed drainage. This result indicates the need for lysimeter outflow measurements to calibrate the Hydrus-1D to simulate water fluxes in evapotranspiration covers.

Examination of the Hydrus-1D indicated a drainage rate of 24.7% and a rate of 75.3% for evapotranspiration for a historical 27-year daily data set, which agree with the measurements and simulations reported in the literature. Lower drainage was estimated when increasing the root depth and crop height. The drainage ranged from 20.7% to 9.9% when using 0.30 and 1.0 m root depth and from 23.7% to 12.9% of the precipitation when the crop height varied from 0.30 to 1.0 m. Likewise, an increase in fine particles, < 2 mm diameter, in the substrates may provide further drainage reduction.

Overall, this study showed that the calibrated Hydrus-1D reproduced consistent drainage and evapotranspiration values for potash tailings covers. Future studies can consider the temporal settling and compaction of the substrates due to the saturation and desaturation processes. These phenomena may provide distinct values for the hydraulic parameters from the technogenic substrates and drainage rates.

Further research can also determine the water fluxes of evapotranspiration covers under different slopes by using two- or three-dimensional models. Moreover, a longer-term observation of drainage from substrates would allow for the validation of the calibrated Hydrus-1D with the experimental data.

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References

Abtew, W., and A. M. Melesse, 2013. *Evaporation and Evapotranspiration. Measurements and Estimations*. London: Springer

Allen, R. G., L. S. Pereira, D. Raes, and M. Smith. 1998. *Crop Evapotranspiration - Guidelines for Computing Crop Water Requirements*. Rome: FAO.

Babalola, O., and R. Lal. 1977. Subsoil gravel horizon and maize root growth. *Plant and Soil*, 46(2): 347-357.

Beckers, E., M. Pichault, W. Pansak, A. Degré, and S. Garré. 2016. Characterization of stony soils' hydraulic conductivity using laboratory and numerical experiments. *Soil Discussions*, 2(2): 1103-1133.

Bilibio, C., C. Schellert, S. Retz, O. Hensel, H. Schmeisky, D. Uteau, and S. Peth. 2017. Water balance assessment of different substrates on potash tailings piles using non-weighable lysimeters. *Journal of Environmental Management*, 196(JUL.1): 633-643.

Bilibio, C. 2018. Evapotranspiration and drainage of potash tailings covers. Ph.D. diss., Department of Agricultural and Biosystems Engineering, University of Kassel, Witzenhausen.

Bilibio, C., S. Retz, C. Schellert, and O. Hensel. 2021. Drainage properties of technosols made of municipal solid waste incineration bottom ash and coal combustion residues on potash-tailings piles: A lysimeter study. *Journal of Cleaner Production*, 279(Jan): 123442.

Blume, H. P., G. W. Brümmer, H. Fleige, R. Horn, E. Kandeler, I. Kögel-Knabner, R. Kretzschmar, K. Stahr, and B. M. Wilke. 2016. *Scheffer/Schachtschabel Soil Science*. **1st ed**. Berlin: Springer

Brakensiek, D. L., W. J. Rawls, and G. R. Stephenson. 1986. Determining the saturated hydraulic conductivity of a soil containing rock fragments. *Drainage Principles and Applications*, 50(3): 834-835.

Cañedo-Argüelles, M., S. Brucet, S. Carrasco, N. Flor-Arnau, M. Ordeix, S. Ponsá, and E. Coring. 2017. Effects of potash mining on river ecosystems: An experimental study. *Environmental Pollution*, 224(MAY): 759-770.

Deutsche Wetterdienst. 2017. DWD Climate Data Center (CDC). Available at: ftp://ftp-cdc.dwd.de/pub/CDC/. Accessed 14 August 2017.

Doorenbos, J., and W. O. Pruitt. 1977. *Guidelines for Predicting Crop Water Requirements*. Rome: FAO.

Field, A. P. 2013. *Discovering Statistics using IBM SPSS Statistics*. **4th ed**. London: SAGE.

Goyal, M. R., and E.W. Harmsen. 2014. *Evapotranspiration. Principles and Applications for Water Management*. Oakville: Apple Academic Press

Hauser, V. L., B. L. Weand, and M. D. Gill. 2001. Natural covers for landfills and buried waste. *Journal of Environmental Engineering*, 127(9): 768-775.

Hauser, V. L., D. M. Gimon, J. V. Bonta, T. A. Howell, R. W. Malone, and J. R. Williams. 2005. Models for hydrologic design of evapotranspiration landfill covers. *Environmental Science and Technology*, 39(18): 7226.

Hauser, V. L. 2009. *Evapotranspiration Covers for Landfills and Waste Sites*. Boca Raton: CRC Press.

Hermsmeyer, D. 2001. Soil physical and hydrological evaluation of aluminum recycling by-product as an infiltration barrier for potash mine tailings. Ph.D. diss., Hanover University, Welfengarten.

Hopmans, J. W. 2010. *Infiltration and Unsaturated Zone*. Burlington: Elsevier Science

Kodešová, R., M. Fér, A. Klement, A. Nikodem, D. Tepl, P. Neuberger, and P. Bure. 2014. Impact of various surface covers on water and thermal regime of Technosol. *Journal of Hydrology*, 519(2014): 2272-2288.

Lal, R., and M. Shukla. 2004. *Principles of Soil Physics*. New York: Taylor and Francis.

Lamb, E. 2015. *A Complete Study of Evapotranspiration*. New York: Callisto Reference.

Li, Y., J. Šimůnek, L. Jing, Z. Zhang, and L. Ni. 2014. Evaluation of water movement and water losses in a direct-seeded-rice field experiment using Hydrus-1D. *Agricultural Water Management*, 142(Aug): 38-46.

Novák, V. 2012. *Evapotranspiration in The Soil-Plant-Atmosphere System. Progress in Soil Scienc*e. London: Springer

Papke, G., and H. Schmeisky. 2013. Rekultivierung von Rückstandshalden der Kaliindustrie. Ergebnisse aus langjährigen wissenschaftlichen Begleituntersuchungen der Begrünungsflächen auf der Kalirückstandshalde Sigmundshall in Bokeloh. Ökologie und Umweltsicherung, Bd. 35/2013, Universität Kassel, Witzenhausen

Papke, G., and H. Schmeisky. 2017. Begrünungskonzept für Kalirückstandshalden im Werra-Gebiet – Stufe II Feldversuch Lysimeterfeld auf der Halde IV in Heringen – Endbericht Teilbericht A. Umweltsicherung Schmeisky, unveröffentlichter Bericht

Radcliffe, D. E., and J. Šimůnek. 2010. *Soil Physics with HYDRUS. Modeling and Applications*. Florida: CRC Press

Rassam, D., J. Šimůnek, and M. Th. Van Genuchten. 2003. *Modelling Variably Saturated Flow with HYDRUS-2D*. Brisbane: ND Consult.

Rauche, H. 2015. Die Kaliindustrie im 21. Jahrhundert. Stand der Technik bei der Rohstoffgewinnung und der Rohstoffaufbereitung sowie bei der Entsorgung der dabei anfallenden Rückstände. (1 Aufl.). Berlin: Springer

Rock, S., B. Myers, and L. Fiedler. 2012. Evapotranspiration (ET) covers. *International Journal of Phytoremediation*, 14(sup1): 1-25.

RStudio Team. 2015. *RStudio. Integrated Development for R*. Boston, MA: RStudio, Inc.

Schaap, M. G., F. J. Leij, and M. Th. Van Genuchten. 2001. Rosetta: A computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions. *Journal of Hydrology*, 251(3-4): 163-176.

Schmeisky, H., and G. Papke. 2013. Begrünungskonzept für Kalirückstandshalden im Werra-Gebiet – Stufe II Feldversuch Lysimeterfeld auf der Halde IV in Heringen - 1. Zwischenbericht Teilbericht A. Umweltsicherung Schmeisky, unveröffentlichter Bericht.

Shukla, M. 2014. *Soil Physics. An Introduction*. Boca Raton: CRC Press.

Šimůnek, J., M. Šejna, H. Saito, M.Sakai, and M. Th. Van Genuchten. 2013. The HYDRUS-1D software package for simulating the movement of water, heat, and multiple solutes in variably saturated media. Version 4.17. Department of Environmental Sciences. Riverside: University of California.

Šimůnek, J., M.Sejna, and M. Th. Van Genuchten. 2014. HYDRUS-1D code for simulating one-dimensional movement of water, heat, and multiple solutes in variably saturated porous media. Available at: https://www.pc-progress.com/. Accessed 13 December 2017.

Šimůnek, J., Van Genuchten, and M.Th., Šejna, M. 2008. Development and Applications of the HYDRUS and STANMOD software packages and related codes. *Vadose Zone Journal*, 7(2): 587-600.

Thornthwaite, C. W. 1948. An approach toward a rational classification of climate. *Geographical Review*, 38(1): 55-94.

Tukimat, N. N. A., S. Harun, and S. Shahid. 2012. Comparison of different methods in estimating potential evapotranspiration at Muda Irrigation Scheme of Malaysia. *Journal of Agriculture and Rural Development in the Tropics and Subtropics*, 113(1): 77-85.

Van Genuchten, M.Th. 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Science Society of America Journal*, 44(5): 892-898.

Van Genuchten, M.Th. 1992. On estimating the hydraulic properties of unsaturated soils. In *Indirect Methods for Estimating The Hydraulic Properties Of Unsaturated Soils.* eds. M.Th. Van Genuchten, F. J. Leij, and L. J. Lund, 1-14. Riverside, CA