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Discussions

Estimating flow and transport parameters in the unsaturated zone with pore water stable isotopes

M. Sprenger[1], **T. H. M. Volkmann**[1], **T. Blume**[2], **and M. Weiler**[1]

[1]Chair of Hydrology, Albert Ludwig University of Freiburg, Freiburg, Germany
[2]GFZ German Research Centre for Geosciences, Potsdam, Germany

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Correspondence to: M. Sprenger (matthias.sprenger@hydrology.uni-freiburg.de)

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Abstract

Determining the soil hydraulic properties is a prerequisite to physically model transient water flow and solute transport in the vadose zone. Estimating these properties by inverse modelling techniques has become more common within the last two decades. While these inverse approaches usually fit simulations to hydrometric data, we expanded the methodology by using independent information about the stable isotope composition of the soil pore water depth profile as a single or additional optimization target. To demonstrate the potential and limits of this approach, we compared the results of three inverse modelling strategies where the fitting targets were (a) pore water isotope concentrations, (b) a combination of pore water isotope concentrations and soil moisture time series, and (c) a two-step approach using first soil moisture data to determine water flow parameters and then the pore water stable isotope concentrations to estimate the solute transport parameters. The analyses were conducted at three study sites with different soil properties and vegetation. The transient unsaturated water flow was simulated by numerically solving the Richards equation with the finite-element code of Hydrus-1D. The transport of deuterium was simulated with the advection-dispersion equation, and the Hydrus code was modified to allow for deuterium loss during evaporation. The Mualem–van Genuchten and the longitudinal dispersivity parameters were determined for two major soil horizons at each site. The results show that approach (a) using only the pore water isotope content cannot substitute hydrometric information to derive parameter sets that reflect the observed soil moisture dynamics, but gives comparable results when the parameter space is constrained by pedotransfer functions. Approaches (b) and (c) using both, the isotope profiles and the soil moisture time series resulted in satisfying model performances and good parameter identifiability. However, approach (b) has the advantage that it considers the isotope data not only for the solute transport parameters, but also for water flow, and thus increases parameter realism. Approaches (b) and (c) both outcompeted simulations run with parameters derived from pedotransfer functions, which did not result

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in satisfying model efficiencies. Overall, parameters based on this new approach that includes isotope data lead to similar model performances regarding the water balance and soil moisture dynamics and better parameter identifiability than the conventional inverse model approaches limited to hydrometric fitting targets. If only data from isotope profiles in combination with textural information is available, the results are still satisfactory. This method has the additional advantage that it will not only allow us to estimate water balance and response times, but also site specific time variant transit times or solute breakthrough within the soil profile.

1 Introduction

1.1 Inverse modelling

Soils play a major role in the water cycle due to their capacity for filtering, buffering and transforming water and solutes between the atmosphere, the ground water and the vegetation cover (Blum, 2005). Soil physical models are widely used to describe water flow and solute transport in the vadose zone, for example to estimate groundwater recharge and the resulting leaching of solutes (e.g. Vanclooster et al., 2004; Christiansen et al., 2006) and the effects of climate variability (Strasser and Mauser, 2001) and climatic extremes (Bormann, 2009, 2012) on the soil water balance. However, determining the crucial model parameters describing the soil hydraulic functions (Gribb et al., 2009) and solute transport remains a challenge because of the pronounced spatial heterogeneity (Corwin et al., 2006). Methods to determine soil hydraulic characteristics include laboratory measurements of the water retention curve or the hydraulic conductivity of a particular soil sample or soil core or pedo-transfer functions based on grain size distributions (Vereecken et al., 2010). Moving beyond the point scale, the inverse model approach allows optimizing the model parameters by fitting model simulations to observed data at the scale of interest (Russo et al., 1991; Durner et al., 1999; Hopmans et al., 2002; Vrugt et al., 2008). These scales range

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from soil column experiments in the lab where water content, matric potentials and outflow were measured and then used for the parameterization of numerical models (e.g. Whisler and Watson, 1968) to the field scale (e.g. Dane and Hruska, 1983).

Extending the inverse modelling approach by using a combination of different types of data as objective functions generally improves parameter identification (Kool et al., 1985; Ritter et al., 2003). For example, a combination of hydrometric and hydrochemical data allows to optimize both the parameters governing water flow and solute transport, while reducing the ill-posedness of inverse problems (Mishra and Parker, 1989; Medina et al., 1990; Russo et al., 1991). Since transient unsaturated flow and solute transport processes are coupled, two possible approaches to the inverse problem were identified: a simultaneous or a sequential approach, in which hydrometric (e.g. soil moisture, matric potential, outflow) and tracer data (e.g. concentrations in the outflow) are used to either determine the soil hydraulic parameters and the transport parameters in parallel or in two steps (Mishra and Parker, 1989). Mishra and Parker (1989) found that the simultaneous optimization yielded lower parameter uncertainties than the sequential method. The simultaneous optimization approach was applied to infer water flow and solute transport parameters from tracer experiments in columns (Inoue et al., 2000) and at the field scale (Jacques et al., 2002; Abbasi et al., 2003a, b). The sequential approach was used in lysimeter studies under natural conditions, with cumulative outflow and its stable isotope concentration serving as objective functions for the water flow (Maciejewski et al., 2006) and transport parameters (Maloszewski et al., 2006).

While soil core/column and lysimeter experiments have the advantage of well-known boundary conditions, their suitability to derive soil properties for predicting field-scale processes is questionable (Russo et al., 1991). Comparative studies showed that the soil physical parameters derived from inverse modelling on the scale of the targeted model application outcompete parameter sets resulting from laboratory experiments (Ritter et al., 2003; Kumar et al., 2010; Kuntz et al., 2011). For the transport parameters, experiments at the field scale are expected to be more representative of the real

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conditions than soil column or lysimeter studies, because of the scale dependency of the longitudinal dispersivity (Vanderborght and Vereecken, 2007). The inverse modelling approach on the field scale generally results in effective parameters, which lump the systems subscale heterogeneity and describe its behaviour at the targeted scale (Pachepsky et al., 2004).

1.2 Pore water stable isotope profiles

As mentioned above, including hydro-chemical data into the inverse modelling approach has distinct advantages. The concentration of stable water isotopes in the stream flow have widely been used to improve calibration and realism of catchment models (e.g. Birkel et al., 2011; Hartmann et al., 2012) and to infer transit times or residence times of catchments (e.g. Maloszewski et al., 1983; McGuire and McDonnell, 2006; Maloszewski et al., 1992; Fenicia et al., 2010; Roa-Garcia and Weiler, 2010; Birkel et al., 2012; Seeger and Weiler, 2014). Similarly, the concentration of stable isotopes in the outflow of lysimeters where used to derive transit times in the vadose zone (Stumpp et al., 2009a, b). However, this type of flow concentration data is not easy to come by at the pedon scale, where we usually are not able to measure breakthrough curves, as we would do in column or lysimeter experiments. One possible solution to this problem is the determination of stable water isotopes (deuterium and oxygen-18) in the pore water. If the isotopic composition of the infiltrating water varies over time, the water transport within a soil profile can thus be traced. Hence, the time dimension of the tracer input (isotopes in the rain over a several year sequence) is preserved in the space dimension (isotopes in the pore water over depth) (Eichler, 1966).

Such pore water stable isotope analyses have shown to give valuable insights into the hydrological processes in the vadose zone of temperate regions: these profiles provide information on the water balance of forest soils (Eichler, 1966; Zimmermann et al., 1966; Blume et al., 1967; Wellings, 1984) and the infiltration and percolation processes (Darling and Bath, 1988; Gazis and Feng, 2004; Koeniger et al., 2010; Thomas et al., 2013), on the influence of vegetation on evaporation (Zimmermann et al., 1967), on

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preferential root water uptake (Gehrels et al., 1998), and on subsurface hydrological processes in hillslopes (Blume et al., 1968; Garvelmann et al., 2012). Despite the high information content of soil water isotope profiles, this type of data has so far not been included in inverse parameter identification approaches for the purpose of vadose zone modelling.

1.3 Objectives

Previous work can be summarized in the following statements which guided the design of our study: (i) a combination of hydrometric and hydro-chemical data decreases ill-posedness of an inverse problem, (ii) parameter optimization/estimation should be conducted on the scale of the application, (iii) determination of pore water stable isotope concentrations allow to track water particles under variable natural boundary conditions over long time spans. As mentioned above, the use of pore water stable isotope profiles for calibration of soil physical parameters for the vadose zone in a humid climate has so far not been rigorously tested. This study will fill this research gap by focusing on three different approaches to include pore water isotope concentrations in an inverse modelling framework and thus answering the following research questions: do stable water isotope profiles as a solitary optimization target provide enough information to derive soil physical and solute transport parameters? Does a combination of pore water isotope profiles and soil moisture time series as parallel optimization targets result in a more adequate parameter representation? Is the sequential use of soil moisture data to determine first the soil physical parameters and using the pore water isotope information to estimate the solute transport parameters afterwards most reliable? The objective of this paper is to investigate these questions in a comparative study applying all optimization approaches to three different sites and thus a range of soil types. The different inverse model approaches that include either pore water stable isotope concentrations alone or in combination with soil moisture data in a parallel or subsequent manner will be compared with regard to the model performances, the

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parameter identifiability and the model realism concerning water balance and transit time estimations.

2 Methods

2.1 Site descriptions and data availability

The inverse model approaches were tested for three study sites located in temperate Central Europe: Roodt, in the West of the Grand Duchy of Luxemburg, and Eichstetten and Hartheim, in the Southwest of Germany. Their environmental characteristics and available data are summarized in Table 1. The three study sites have a similar climate, with rainfall occurring all year with mean precipitation between 660 to 900 mm yr^{-1}. However, the study sites differ in their geological and pedological setting. The soil in Roodt is a Cambisol characterized by a ploughed humous mineral horizon (Ap) in the upper 25 cm, followed by a loamy brown B-horizon (Bv) over heavily weathered schist rocks (stone content > 80 %; Cv) starting in 50 cm soil depth. In Eichstetten, the prevailing soil is a slightly clayey silt Luvisol, developed on pleistocene aeolian loess (Hädrich and Stahr, 2001). In Hartheim, the soil is a Calcaric Regosol with a silty sandy top soil (> 40 cm) on fluvial gravel and coarse sand (Schäfer, 1977). The study sites in Roodt and Eichstetten are grasslands and the site in Hartheim is a Scots pine plantation (*Pinus sylvestris*). All three sites are located on undulating terrain, where vertical flow is dominating and lateral subsurface flows can be neglected.

The data availability varied between the study sites. The sites in Roodt and Eichstetten had continuous soil moisture measurements that were averaged to daily values, whereas in Hartheim, the soil moisture was determined destructively with soil cores taken weekly and in exceptions bi-weekly to three-weekly. The methodology for the pore water isotope measurements differed for the different study sites, due to the technical possibilities at the time of the sampling. At the sites in Roodt and Eichstetten, the soil samples were taken during the years 2012 and 2013 and analysed for their pore

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water isotopic composition according to the equilibration method (Wassenaar et al., 2008). Each isotope profile was determined by taking soil samples in 5 cm depth intervals from a soil core excavated with a percussion drill (Atlas Copco Cobra). The soil samples were taken to the laboratory in sealed air-tight bags. In addition to the soil samples, standards were prepared, which consisted of oven-dried soil material that was rewetted to the soil moisture at the time of sampling with three different waters of known isotopic composition. After adding dry air to both, standards and field samples, the bags were re-sealed. The soil pore water was allowed to equilibrate with the dry atmosphere in the bag for two days under constant temperature (21 °C). The headspace in the bags was directly sampled with a Wavelength-Scanned Cavity Ring Down Spectrometer (Picarro, Santa Clara, USA) for 6 min, and only the measured concentration of deuterium and ^{18}O during the last 90 s was averaged to minimize carryover effects. The isotopic composition of the gas phase was converted to values of the liquid pore water according to the temperature dependent fractionation factor as defined by Majoube (1971). The standards were measured at the beginning, every three hours during, and at the end of the analysis for each profile. The standards were used to account for drift of the laser spectrometer and to calibrate the measurements in order to get values in the δ notation relative to the Vienna Standard Mean Ocean Water (VSMOW). The measurement accuracy, given as the average range of repeated measurements of the standards over the day, was 1.96 ‰ for δ Deuterium. At the Hartheim site, the sampling took place in 1999 and 2000 and the pore water isotope analysis was done by excavating 500 g of soil in 5 cm intervals and extracting the pore water with the means of azeotropic distillation with toluol (Revesz and Woods, 1990). The extracted pore water was then analysed for the deuterium concentration with a mass spectrometer (Finnigan MAT-DeltaS, Bremen, Germany).

Precipitation was measured either above the canopy (Hartheim) or in the open field (Roodt, Eichstetten). The isotopic composition of the rainfall in Roodt and Eichstetten and throughfall in Hartheim was determined at the study sites at least 14 months before the isotope profile sampling started and then at least every 14 days. The rainwater

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isotope analyses were done with the same equipment as the pore water analysis. To minimize the influence of the initial conditions of the deuterium concentration in the pore water, the time series of isotope concentration of the precipitation were extended with additional isotope data from other sampling locations close by.

2.2 Model setup

2.2.1 Water transport

The transient water flow within the unsaturated soil profile was simulated by numerically solving the Richards equation with the finite-element code of Hydrus-1D (Šimůnek et al., 2012). For the parameterization of the water retention ($\Theta(h)$) and the unsaturated hydraulic conductivity ($K(h)$) functions, the Mualem–van Genuchten model (van Genuchten, 1980) was applied. These relations are specified by the residual and saturated volumetric water contents (θ_r [$L^3\,L^{-3}$] and θ_s [$L^3\,L^{-3}$], respectively), the inverse of the capillary fringe thickness (α [L^{-1}]), two shape parameters (n [–], and m [–], where $m = 1 - 1/n$), the saturated hydraulic conductivity (K_s [$L\,T^{-1}$]), and a tortuosity parameter (l [–], in accordance to Mualem (1976) set to 0.5 to reduce the number of free parameters).

A sink term in the Richards equation was defined according to the root water uptake model by Feddes et al. (1978), which describes the reduction of the potential water uptake by a dimensionless trapezoidal stress response function. Such non-optimal conditions for the vegetation are defined by pressure heads above and below which the plants experience oxygen or water stress, respectively. In this study, the following prescribed parameter set for pasture (Wesseling, 1991) was used for all sites, since no parameter for scots pine are available: > -10 cm oxygen stress occurs; between -25 and -800 cm optimum; below -8000 cm root water uptake ceases. The root water uptake was restricted to the root zone, which was defined by the sites' specific rooting depth (20, 30, and 40 cm for Roodt, Eichstetten, and Hartheim, respectively) and a root distribution according to Hoffman and van Genuchten (1983).

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The potential evapotranspiration (PET) was estimated with the Hargreaves Formula as a function of extraterrestrial radiation and daily maximum and minimum air temperature. The PET was split into potential evaporation and potential transpiration according to Beer's Law (Ritchie, 1972), which is a function of the leaf area index (LAI) and the canopy radiation extinction factor (set to 0.463).

To assess the seasonal variability of the LAI in the grassland sites (Roodt and Eichstetten), the year was divided into winter season (1 November–1 March, LAI = 0.2, Breuer et al., 2003) and summer season (1 May–1 September, LAI = 2). In the transition period between the two seasons, the LAI was linearly interpolated. The interception of precipitation was considered at the grassland sites as a function of the precipitation, LAI and an empirical constant (set to 0.55 mm, which results in a maximum of 1.1 mm interception for a LAI of 2). In the scots pine forest in Hartheim, the annual average throughfall was set to be about 2/3 of the precipitation at a constant LAI of 2.8, both as reported by Jaeger and Kessler (1996). The snow module developed by Jarvis (1994) was included, where precipitation falls as snow for air temperatures $< -2\,^{\circ}C$ and as rain for temperatures $> +2\,^{\circ}C$. Between -2 and $+2\,^{\circ}C$ the percentage of snow in precipitation decreases linearly. For snow that accumulated at the soil surface, the degree-day method was applied. The required constant, which describes the amount of snowmelt during one day for each $^{\circ}C$ above zero, was set to 0.43 cm d^{-1} K^{-1}.

2.2.2 Deuterium transport

To account for the isotopic composition of the soil water, the concentration of deuterium was simulated as a solute in the Hydrus model. Since the model originally was not developed to include stable isotope modelling, a modified version of Hydrus was used, which was introduced by Stumpp et al. (2012) and allows for solute losses caused by evaporation. This modification prevents an accumulation of the deuterium concentration at the upper boundary. The δ notation, in ‰ VSMOW of the isotopic concentration was used for calculating the isotopic compositions and its mixing.

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Isotopic enrichment due to fractionation processes during evaporation was not included in the model. This assumption was considered to have a minor impact on the simulations, because the deuterium-^{18}O relationship of the pore waters at the study sites were similar to the global meteoric water line (GMWL), suggesting limited effects of isotope enrichment. Furthermore, Maloszewski et al. (2006) found in a similar climate that the average deuterium contents in precipitation and the water outflow of a lysimeter in −200 cm depth were nearly the same, concluding that fractionation due to evaporation does not play a big role in temperate climates.

Within the Hydrus code, the deuterium transport was calculated according to the advection-dispersion model, which is the most widely used model to predict solute transport in soils under field conditions (Vanderborght and Vereecken, 2007). The advective part of that equation is governed by the mean water flux. The dispersion term represents the hydro-chemical dispersion and the molecular diffusion. The former is a function of the longitudinal dispersivity λ [L], the water content θ [$L^3 L^{-3}$], and the water flux q [$L T^{-1}$], while the latter is governed by the molecular diffusion coefficient in free water D_w [$L^2 T^{-1}$] (2.272×10^{-9} $m^2 s^{-1}$ according to Mills, 1973) and a tortuosity factor τ_w [–] as defined by Millington and Quirk (1961). As deuterium is part of the water molecule it can leave the soil profile via evaporation at the soil surface or via root water uptake.

The profiles have been discretized into 101 nodes, with higher node density at the top than at the bottom to enhance model stability. The soil profiles were discretized into two different horizons according to the soil descriptions in (Table 1). The depth of the simulation was 200 cm for Roodt and Eichstetten and 120 cm for Hartheim.

2.2.3 Initial and boundary conditions

The site-specific initial conditions were defined by a constant water content ($0.2\ cm^3\ cm^{-3}$) and a constant pore water deuterium concentration, representing the weighted average concentration in precipitation (−54, −60, and −56 ‰ for Roodt, Eichstetten, and Hartheim, respectively). The influence of the initial conditions on the

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calibration can be neglected, as a spin-up period of at least two years was simulated before the start of the calibration period. The upper boundary condition was defined by variable atmospheric conditions (Cauchy boundary condition) that govern the loss of water and deuterium caused by evapotranspiration, the input of water due to throughfall and the accompanied flux concentrations of deuterium. The lower boundary was set to zero-gradient with free drainage of water and solutes.

2.2.4 Parameter optimization and sensitivity

Six parameters had to be optimized for each horizon of the soil profiles to simulate the water and solute transport in the unsaturated zone. On the one hand the five parameters θ_r, θ_s, α, n, K_s, describing the water retention and hydraulic conductivity characteristics in accordance to the Mualem–van Genuchten model (MVG) were determined. In addition, the longitudinal dispersivity λ, describing the dispersion of the deuterium, was subject to the optimization process. The ranges of the parameter space are listed in Table 2. To find the global optima of the parameter space that best simulates the observed data, the Shuffled-Complex-Evolution algorithm (SCE-UA) developed by Duan et al. (1992) was applied. The search algorithm terminates when the objective function does not improve by > 0.01 % within 10 evolution loops. The number of complexes used by the algorithm was defined as the number of optimizing parameters minus three, but not higher than eight or lower than three. All other parameters that govern the optimization algorithm were chosen as recommended by Duan et al. (1994). The modified Kling–Gupta-Efficiency (KGE) as defined by Kling et al. (2012) was applied as the objective function in the optimization process. The dimensionless KGE compares simulated and observed data with regard to their correlation r, their ratio of the mean values (bias ratio, β), and their ratio of the coefficient of variation (variability ratio, γ) as follows: $\mathrm{KGE} = 1-[(1-r)^2+(1-\beta)^2+(1-\gamma)^2]^{0.5}$. For parameter combinations that did not lead to a numerical convergence of the Hydrus code, a high value of the objective function was assigned. This method, as suggested by Wöhling et al. (2008), prevents the SCE-UA algorithm from searching for an optimum in an unrealistic parameter space.

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A KGE was computed for each soil moisture time series at the various depths and an average KGE_θ, weighted by the number of data points for each depth was calculated to get a representative KGE for the soil moisture across the profile. Similarly, a KGE was calculated for each isotope profile and an average efficiency was derived from the mean value of all profiles (KGE_D).

The following three different inverse model approaches were tested:

1. The isotope profile approach (IPA): only the observed pore water isotope profiles were considered in the objective function. The MVG and dispersivity parameters were all optimized in a way to reflect the observed pore water deuterium concentrations in the profiles (KGE_D as objective function). The initial parameter ranges were constrained by pedotranfer functions using the observed soil texture (Table 1). After determining the soil texture for each horizons, the surrounding neighbours in the textural triangle were determined and the corresponding MVG parameters were derived with the Rosetta PTF (Schaap et al., 2001). The range of the MVG parameter values of the neighbouring textural classes defined the parameter range in which the IPA was allowed to search for an optimal parameter set. Also a variant, where the parameter space of the MVG was unconstrained was tested (uIPA).

2. The multi-objective approach (MOA): the measured soil moisture time series and isotope profiles were used to simultaneously optimize the parameter for the water and deuterium transport. Both fitting targets were equally balanced, because the KGE was calculated from the average over the efficiencies of the simulated soil moisture series and the isotope profiles ($KGE_{tot} = (KGE_\theta + KGE_D)/2$).

3. The two-step approach (2SA): the MVG parameters were optimized first by minimizing the difference between observed and simulated soil moisture (KGE_θ). Afterwards, these MVG parameters were applied in order to optimize the dispersivity parameter using the observed isotope profiles (KGE_D).

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In addition to the inverse model approaches, the efficiency of the simulations with parameter sets derived from pedotransfer functions (PTFs) were also tested. The Rosetta PTF (Schaap et al., 2001) was used to estimate the MVG parameters from soil textural information of the horizons. As Rosetta does not account for the dispersivity, it was either estimated by an additional PTF (Perfect et al., 2002) or again optimized using the isotope profile.

The sensitivities of the model to the individual parameters of the different inverse modelling approaches were compared with the Regional Sensitivity Analysis (RSA) introduced by Spear and Hornberger (1980) and Hornberger and Spear (1983). For each optimization approach and study site, the cumulative probability distribution of the parameter set of the best performing 10 % of model runs during the optimization process was considered for the sensitivity analysis. Of this selection the 10 to 90 percentile range ($PR_{10–90}$) was calculated for each parameter as a measure for the sensitivity. Since the boundary of the possible parameter space was narrowed down in the IPA via PTFs, but unconstrained in the other approaches, the $PR_{10–90}$ was normalized by the range of the parameter space. Hence, the $PR_{10–90}$ represents the normalized parameter ranges between the 10th and the 90th percentile of the 10 % best optimization runs as a percentage of the initial boundaries of the parameter space. As the search algorithm modulation is the same for every study site and optimization approach, the $PR_{10–90}$ allows for a comparison of the relative parameter sensitivity of the different approaches.

2.3 Water balance and transit time calculations

For each inverse modelling approach and study site, the parameter combination that resulted in the highest model efficiency (Table 3) were used in a forward model approach to reveal the consequences for water balance and transit time calculations. The cumulative annual water balance from daily seepage and evapotranspiration losses were computed over six years for each study site. To infer transit times through the soil profiles rain input was traced virtually for two events of intermediate intensities

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(between 8 and 13 mm day^{-1}), one at the beginning of October (called "fall event") and one at the beginning of May (called "spring event").

3 Results

3.1 Model performance for soil moisture and pore water isotopes

The simulations with the parameter sets derived with the unconstrained isotope profile approach (uIPA) did not reproduce the soil moisture dynamics at any of the sites in a satisfactory manner (Fig. 1). The values of the KGE_θ, which did not serve as an objective function in the uIPA, ranged between −0.35 and 0.10 for the three different sites (Table 3). The models generally underestimated the water content in the upper soil layer, whereas for Roodt and Eichstetten, the model overestimated the water content for the lower layers (at Hartheim there were no soil moisture measurements in the lower layer). For Hartheim, the high variation of the weekly measured data was not met by the simulations, but the mean of the series was reproduced. The model performance regarding the soil moisture dynamics was increased due to a constrained initial parameter space via PTFs in the IPA by 0.19, 0.61, and 0.14 for Roodt, Eichstetten and Hartheim, respectively. The IPA resulted in simulations reflecting the general pattern of the seasonal soil moisture changes. However, the other two approaches (MOA and 2SA), which included the soil moisture data in the parameterization, performed better in simulating the temporal dynamics of water contents in the soil profiles. For Roodt and Eichstetten, the KGE_θ were above 0.7 and the residuals were within the uncertainty range of the sensors (±0.03 cm^3 cm^{-3}) except for dry periods in Eichstetten. For Roodt, where the observed soil moisture time series are averages of three sensors per depth, the deviation of the three sensors from their average value was higher (0.03 to 0.08 cm^3 cm^{-3}) than the residuals of the simulations of MOA and 2SA. The model efficiency for soil moisture dynamics at Hartheim is lower than for the other study sites (KGE_θ 0.20 and 0.42 for the MOA and the 2SA, respectively). The modelled soil

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moisture data with the best parameter set of MOA does not reflect the temporal variability of the observed data, but the mean values are reproduced. With the parameter set resulting from the 2SA, the dynamics, as represented by the coefficient of variation in the KGE, are better simulated, but the correlation between observed and simulated data is lower.

For the pore water deuterium concentrations, the best fits with KGE_D between 0.72 and 0.86 were achieved with the parameters derived from uIPA (Fig. 2 and Table 3). Constraining the parameter space (IPA) led to a decrease of the KGE_D by 0.07 to 0.11. Including soil moisture data into the calibration (MOA) reduced the KGE_D moderately to values between 0.67 and 0.81. Parameters derived with the 2SA resulted in slightly lower model efficiency at Roodt and Eichstetten with a KGE_D of 0.62 and 0.79, respectively. For Hartheim, the 2SA resulted in the lowest KGE_D of 0.40. The fit between simulated and observed pore water isotope concentrations is not equally good for all the sampling times at the same sampling site. For Roodt, the isotope profile from October was better simulated than the profile sampled in March. While the peak of isotopically enriched water from summer precipitation in 30 to 50 cm soil depth is well simulated in the October profile, there is a higher vertical variability in the simulated profile than in the observations. For Eichstetten, the isotope profile in November was reproduced more closely than the ones taken in January and March. Temporal dynamics of the model fit are less pronounced for the site in Hartheim, where the vertical variability across the soil profile is generally lower than at the other two study sites. Estimating the MVG parameter with the Rosetta pedotransfer function (PTF) (Schaap et al., 2001) via textural information at Roodt and Eichstetten, did not result in a proper representation of the soil moisture dynamics (KGE_θ of 0.03 and 0.27, respectively). Using the texturally dependent PTF for the dispersivity parameters (Perfect et al., 2002) in combination with the MVG parameters from the Rosetta PTF failed to simulate the measured pore water isotope concentrations in Roodt ($KGE_D = -0.14$), while the result for Eichstetten was better ($KGE_D = 0.53$). An inverse estimation of the dispersivity parameter with KGE_D as the objective function while using the MVG of the Rosetta PTF

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resulted in higher model efficiencies as with the dispersivity parameters derived from the PTF of Perfect et al. (2002). However, the efficiencies were much lower than for the three presented inverse model approaches, with KGE_D of 0.18 and 0.59 for Roodt and Eichstetten, respectively.

3.2 Parameter sensitivity

The sensitivity analysis based on the 10–90 percentile ranges of the 10 % best parameter sets showed that the uIPA results in least identifiable parameters for Roodt and Eichstetten, while the MOA gives the best results regarding the parameter sensitivity (Fig. 3). The $PR_{10–90}$ values of the uIPA are at least 4 and 2 times higher than for the MOA at Roodt and Eichstetten, respectively. The sensitivities of the parameters from the 2SA take an intermediate position, where the K_s parameters show lowest sensitivities ($PR_{10–90}$ 10 to 16 % for Roodt and Eichstetten, respectively). For Hartheim the pattern in the relationship between optimization approach and parameter sensitivities is less pronounced and the MOA does not result in the best identifiable parameters. At this site only, the 2SA results in a substantial difference in sensitivities between the upper and lower layer: MVG parameters of horizon 1 (except for α) have 3 to 23 times lower $PR_{10–90}$ values than the parameters of horizon 2. In general, K_s shows the lowest sensitivities for all sites and optimization approaches (more than half of the $PR_{10–90}$ values are above 5 %, respectively), while θ_r, and θ_s are of immediate sensitivities (1/3 of the $PR_{10–90}$ are > 5 %) and both α and n are usually well identified (1/4 and 1/5 of the $PR_{10–90}$ values are > 5 %, respectively).

The water retention curves and the unsaturated hydraulic conductivity for Roodt and Eichstetten are similar for the MOA and the 2SA, while the IPA and especially the uIPA yielded parameter combinations that result in rather different retention curves (Fig. 4 and Table 4). This pattern is less pronounced for the different inverse modelling approaches for Hartheim. For Roodt, the dispersivity is higher in the upper layer, while it is higher in the lower layer for Eichstetten and Hartheim using the MOA and 2SA (Table 4).

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3.3 Consequences for the water balance and water transit times

Magnitudes of site-specific water balance components derived with the MOA and 2SA are generally of similar range (Fig. 5). The water balance components derived with the uIPA deviate from the other inverse modelling approaches resulting in high seepage fluxes and low evapotranspiration for Roodt and Hartheim. These high seepage rates, which are twice as high as the ET for Eichstetten, are due to the high hydraulic conductivities in the upper soil horizon estimated by the uIPA. The water balance simulated with the uIPA for Eichstetten is not realistic, since the annual ET is reported to be about 80 % of the precipitation (ET/P = 0.8) in this region (upper Rhine Valley) (Wenzel et al., 1997). In contrast, the IPA, MOA and 2SA result in an ET/P between 0.77 and 0.82 for three of the four simulated years. For Hartheim the simulated ET/P ratios are with 0.63 to 0.85 in a similar range as derived from latent heat flux estimates (ET/P = 0.71 to 0.88) for the years 2000 and 2001 (Imbery, 2005).

The fact that parameters derived with the different optimization approaches differ less for Roodt and Hartheim than for Eichstetten is also reflected in the results of the transit time estimations. Cumulative breakthrough curves of the traced event waters leaving the soil profile at the lower boundary were determined for two events (Fig. 6). Figure 6 does not only visualize the timing and amount of event water in the seepage flux, but also the fraction of seepage water to ET (i.e. difference to unity). There are pronounced seasonal effects with at least four times higher seepage-ET ratios for the rain event in fall than for the spring event. In general, precipitation in fall is more likely to leave the soil via seepage and to do so after shorter transit times. Big differences between the approaches were found for Eichstetten, where transit times are twice as long for the IPA, MOA and the 2SA than for the uIPA, respectively. For Roodt, transit times of the IPA and uIPA were about double as long as for the MOA and 2SA.

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4 Discussion

4.1 Parameter adequacy

The MOA shows highest overall parameter adequacy when challenging the results of the conducted model calibrations in accordance to Gupta et al. (2006) with regard to: (i) the fit between observed and simulated data, (ii) accuracy of the parameter sets, and (iii) consistency of the model behaviour. The MOA outcompetes the other inverse model approaches with respect to the overall efficiency (KGE_{tot}) of the simulation of both the soil moisture dynamics and pore water isotope concentrations (Table 3): parameter identifiability is the highest and the simulated water balance components and transit times are in line with the understanding of the processes at the study sites. The 2SA gave satisfactory results in the model efficiencies and model consistencies, but showed weaknesses regarding the identifiability of the parameters due to the fact that five MVG parameters for two horizons were optimized with just one objective function (KGE_{θ}) in the first step. The uIPA, where also just one objective function was applied (KGE_D), showed problems with respect to the identifiability as well as low model performance and realism. The identifiability of the IPA appears to be well in Fig. 3, but caution has to be paid since some parameters moved to the boundaries of the parameter space set by the Rosetta PTF, resulting in little or no changes within the best performing 10 % of the optimization runs (e.g. for Roodt 7 out of the 12 parameters reached boundaries). All parameters that moved to the boundaries during the optimization with the IPA are indicated with a star in Table 4. Despite this limitation, the IPA reveals that the information about soil texture to limit the possible parameter range helps to find an overall more realistic parameter set. Constraining the possible parameter space of the MVG parameters resulted in increased KGE_{tot}, while the objective function of the IPA resulted in slightly lower values.

The inadequate representation of the soil moisture dynamics using the soil physical parameters derived with the Rosetta PTF shows that site-specific hydrological characteristics can hardly be reflected via textural information. Nevertheless, soil structure

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has to be taken into account. This is especially true for Roodt, where a high rock content influences the water flow. The fact that the soil moisture simulations as well as the pore water isotope simulations with parameters derived via the PTF are better for Eichstetten, where a more homogenous soil prevails than in Roodt, supports the idea that the application of PTFs require homogenous flow through the soil matrix. In general the KGE_{tot} was lower in the approaches that made use of PTF than for the MOA and the 2SA, which shows the advantage of inverse modelling in effectively and site specifically optimizing the model parameters. Our findings support the acknowledged fact that PTFs have a limited transferability from the region and scale they were developed, since they do not account for the pore structure (Pachepsky et al., 2006). Even though the soil is not a homogenous porous medium as assumed for the applied Richards equation, our simulations of water flow and isotope transport on daily resolution over several years seems to capture the hydrological processes of percolation, evapotranspiration and dispersion of pore waters reasonably well. Highest deviations of the modelled soil moisture dynamics from the observed data are found during dry periods. The overestimation of the water content in these cases is likely caused by the simplified root distribution and water uptake model.

4.2 Dispersivity parameter estimation

An increase of the dispersivity parameter with depth and length, as found in several core-, column-, and lysimeter experiments (summarized by Pachepsky et al., 2000, and Vanderborght and Vereecken, 2007) was only found for Eichstetten. For Roodt and Hartheim, the dispersivity was higher in the upper horizon. However, the scale dependency of the dispersivity is generally reported to be less pronounced or non-existent for the field scale experiments and longer travel distances (Vanderborght and Vereecken, 2007). The estimated values for the dispersivity parameters are mostly within the range (0.8–20 cm) as reported in a review by Vanderborght and Vereecken (2007) for the field scale. However, the results of the dispersivity parameters derived by the MOA and 2SA for Roodt and Eichstetten (0.12–9 cm), which can be seen as

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most reliable simulations, are at the lower end of the data presented in the review by Vanderborght and Vereecken (2007) and lysimeter studies by Stumpp et al. (2009a, 2012). As the dispersivity parameter was shown to be scale dependent (Vanderborght and Vereecken, 2007), the presented methodology provides the opportunity to optimize parameters for each soil horizon, in contrast to soil column or lysimeter studies, where the dispersivity parameter is integrated over the entire soil profile (Inoue et al., 2000; Stumpp et al., 2012). In addition, only 1 to 2 sampling campaigns are necessary to get the additional information for water and solute transport. The high variability of the dispersivity between the sites and horizons in our study and reported in other studies (Vanderborght and Vereecken, 2007) and the limited model efficiencies when PTFs were applied emphasize the importance to consider this solute transport parameter in the parameterization of soil physical models. Thus, a field scale representation of the dispersion processes can therefore not be assumed for a certain soil texture, but must be derived for the particular field site. The fact that the soil moisture sampling at Hartheim was constrained to the upper soil layer but pore water isotope data reached to depth of 120 cm explains the large differences between MOA and 2SA at that study site. The MVG parameters of the lower layer are in this case non-identifiable. Nevertheless, the MOA results in reasonable simulations of the soil moisture and the isotope profiles in Hartheim.

4.3 Advantages of multi-objective approaches

Our comparative study supports the findings by others that the more data types are taken into account during the calibration process, the lower is the model's performance with respect to different specific objective functions. For catchment models it has been shown that including stream water chloride (Kuczera and Mroczkowski, 1998) or isotope concentrations (Fenicia et al., 2008; Hartmann et al., 2012) in the optimization process reduced stream discharge simulation efficiency, but increased model realism and parameter identifiability. On a different scale, a similar effect was reported for soil physical models, as shown in comparative studies, where soil moisture data from soil

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cores were combined with pressure heads (Zhang et al., 2003; Vrugt and Bouten, 2002) or with leachate volume of lysimeters (Mertens et al., 2006) to increase identifiability. Our study is in line with these findings, but expanded the comparison to the field scale and included hydrochemical data. The simultaneous optimization outcompeted the two-step optimization with regard to identifiability (as also found by Mishra and Parker, 1989), while providing similar overall performance as the 2SA. The MOA has the advantage that the MVG parameters are additionally constrained by the percolation velocity in the advection-dispersion function used to simulate the isotope profile, and not just by the soil moisture dynamics, as for the 2SA. Another advantage is the lower time requirement for the calibration using MOA, because the parameterization is done in one and not in two subsequent steps. Considering these advantages, with a performance that is as good as for the 2SA, and much better than the IPA and uIPA, the MOA represents the best inverse model approach. These findings are in line with Mishra and Parker (1989), who also found the simultaneous estimation of hydraulic and transport properties to be better than the sequential inversion of first hydraulic properties from water content and matric pressure head data, followed by inversion of transport properties from concentration data. Inoue et al. (2000) also showed a successful application of the simultaneous optimization of soil hydraulic and solute transport parameters, but did not compare the performance with a two-step optimization. In accordance to our findings that the KGE_θ was only slightly lower for the MOA than for the 2SA (Table 3), Abbasi et al. (2003a) found a better performance for the simulation of the soil moisture data when the two-step approach was applied. However, with respect to drainage rates and concentrations, the simultaneous optimization of the water flow and solute transport parameters resulted in as good model performances as the sequential approach (Abbasi et al., 2003a; Jacques et al., 2002). In our study, we aimed to represent the water flow and isotope transport on the pedon scale as complex as needed, but as simple as possible. Therefore, processes like preferential flow, hysteresis or mobile–immobile interactions in the soil were not considered. Including these processes in the model would cause a need for more parameters, which is likely to result in lower identifiability.

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However, even in this case the additional isotope data may help to better constrain the parameters.

4.4 Transit time estimations

There is an additional benefit in taking isotope data into consideration in soil physical models with respect to the possibility of tracing the water movement through the soil. The fact that the pore water isotope data allows us to determine the dispersion of the water during the percolation processes provides the opportunity to apply particle tracking of the precipitation water. As a consequence, the presented inverse model approaches that include the water's isotopic signal on the field scale outcompete the usually applied parameterization of soil physical models that consider only hydrometric data. By simulating the isotope transport in the unsaturated zone, not only the response time, but also the transit time of the water can be predicted, which provides additional valuable information for a better understanding of the hydrological processes in the subsurface. The approach is limited to environments where a seasonal variation in the isotopic composition of precipitation exists and soil evaporation and thus isotopic fractionation processes play a minor role. However, isotope fractionation processes due to evaporation could also be included in a Richards based model. The presented inverse model approaches including the estimation of the dispersivity parameter at the field scale will be beneficial for studies dealing with pollutant and nutrient transport through the soil.

5 Conclusions

We conclude that the information gained by the snap shot sampling of soil water isotope profiles allows for a more realistic parameterization of soil physical models. Our study showed the strength of pore water isotope information as fitting target for the parameterization of soil physical models. Stable water isotope profiles as the only optimization

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target (uIPA) do not provide sufficient information to derive soil physical parameters that can reflect the soil moisture dynamics, but constraining the possible parameter space of the MVG parameters with information about the soil texture (IPA) helps to increase model realism. Continuous measurements of the water content or the matric potential seem to be still beneficial for understanding the water movement within the soil profile. Regarding water balance and transit time simulations, the uIPA and IPA have to be applied with caution and model realism has to be tested, for example by field measurements of ET and/or soil storage changes. Since the identifiability is higher for the MOA than for the 2SA, while the model performance and realism are similar, the combination of pore water isotope profiles and soil moisture time series as parallel optimization targets (MOA) result in the most adequate parameter representation. Parameters derived via PTFs did not lead to satisfying simulations.

In general, the consideration of the isotopic signal enables an estimation of the dispersion of the water during the percolation through the soil. As such, tracking of the infiltrated water is possible, which gives insights into the transit times – and not just the response times – of the soil water on the field scale. Hence, isotope profiles in combination with soil moisture time series feature the opportunity to derive time-varying, site-specific transit time distributions of the vadose zone via soil physical models. Although the information is limited to point measurements, a better knowledge of the water velocities and mixing processes will help to benchmark conceptual catchment models. It seems even possible to realistically estimate soil hydraulic parameters from pore water stable isotope profiles alone. This will reduce the time and effort for long-term soil water content measurements significantly, since only one to two sampling campaigns to extract soil samples are necessary.

Tackling the limitations of the here presented study by including preferential flow and isotopic fractionation due to evaporation would open up additional avenues such as estimating the impact of heavy precipitation events and resulting preferential flow on the water and solute transport or differentiating between evaporated and transpired soil water. Overall, we expect the more realistic parameterization of soil physical models based

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on the inclusion of pore water isotope data to improve the assessment of groundwater pollution by water soluble nutrients, pesticides or contaminants.

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References

Abbasi, F., Jacques, D., Simunek, J., Feyen, J., and van Genuchten, M. T.: Inverse estimation of soil hydraulic and solute transport parameters from transient field experiments: heterogeneous soil, T. ASAE, 46, 1097–1111, 2003a.

Abbasi, F., Simunek, J., Feyen, J., van Genuchten, M. T., and Shouse, P. J.: Simultaneous inverse estimation of soil hydraulic and solute transport parameters from transient field experiments: homogeneous soil, T. ASAE, 46, 1085–1095, 2003b.

Birkel, C., Tetzlaff, D., Dunn, S. M., and Soulsby, C.: Using lumped conceptual rainfall–runoff models to simulate daily isotope variability with fractionation in a nested mesoscale catchment, Adv. Water Resour., 34, 383–394, doi:10.1016/j.advwatres.2010.12.006, 2011.

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Birkel, C., Soulsby, C., Tetzlaff, D., Dunn, S., and Spezia, L.: High-frequency storm event isotope sampling reveals time-variant transit time distributions and influence of diurnal cycles, Hydrol. Process., 26, 308–316, doi:10.1002/hyp.8210, 2012.

Blum, W. E. H.: Functions of soil for society and the environment, Rev. Environ. Sci. Biotechnol., 4, 75–79, doi:10.1007/s11157-005-2236-x, 2005.

Blume, H.-P., Zimmermann, U., and Münnich, K.: Tritium tagging of soil moisture: the water balance of forest soils, in: Isotope and Radiation Techniques in Soil Physics and Irrigation Studies, IAEA, Istanbul, 12–16 June 1967, International Atomic Energy Agency, Vienna, 315–332, 1967.

Blume, H.-P., Münnich, K.-O., and Zimmermann, U.: Untersuchungen der lateralen Wasserbewegung in ungesättigten Böden, Z. Pflanz. Bodenkunde, 121, 231–245, doi:10.1002/jpln.19681210307, 1968.

Bormann, H.: Analysis of possible impacts of climate change on the hydrological regimes of different regions in Germany, Adv. Geosci., 21, 3–11, doi:10.5194/adgeo-21-3-2009, 2009.

Bormann, H.: Assessing the soil texture-specific sensitivity of simulated soil moisture to projected climate change by SVAT modelling, Geoderma, 185–186, 73–83, doi:10.1016/j.geoderma.2012.03.021, 2012.

Breuer, L., Eckhardt, K., and Frede, H.-G.: Plant parameter values for models in temperate climates, Ecol. Model., 169, 237–293, doi:10.1016/S0304-3800(03)00274-6, 2003.

Christiansen, J. R., Elberling, B., and Jansson, P.-E.: Modelling water balance and nitrate leaching in temperate Norway spruce and beech forests located on the same soil type with the CoupModel, Forest Ecol. Manag., 237, 545–556, doi:10.1016/j.foreco.2006.09.090, 2006.

Corwin, D. L., Hopmans, J., and de Rooij, G. H.: From field- to landscape-scale vadose zone processes: scale issues, modeling, and monitoring, Vadose Zone J., 5, 129–139, doi:10.2136/vzj2006.0004, 2006.

Dane, J. H. and Hruska, S.: In-situ determination of soil hydraulic properties during drainage, Soil Sci. Soc. Am. J., 47, 619–624, doi:10.2136/sssaj1983.03615995004700040001x, 1983.

Darling, W. and Bath, A.: A stable isotope study of recharge processes in the English Chalk, J. Hydrol., 101, 31–46, doi:10.1016/0022-1694(88)90026-1, 1988.

Duan, Q., Sorooshian, S., and Gupta, V.: Effective and efficient global optimization for conceptual rainfall–runoff models, Water Resour. Res., 28, 1015–1031, doi:10.1029/91WR02985, 1992.

HESSD
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Duan, Q., Sorooshian, S., and Gupta, V. K.: Optimal use of the SCE-UA global optimization method for calibrating watershed models, J. Hydrol., 158, 265–284, 1994.
Durner, W., Schultze, B., and Zurmühl, T.: State-of-the-art in inverse modeling of inflow/outflow experiments, Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, in: Proc. Int. Workshop on Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, edited by: van Genuchten, R., Leij, F., and Wu, L., 22–24 October 1997, Riverside, CA, 661–681, 1999.
Eichler, R.: Deuterium-Isotopengeochemie des Grund- und Oberflächenwassers, Geol. Rundsch., 55, 144–159, doi:10.1007/BF01982963, 1966.
Feddes, R. A., Kowalik, P. J., and Zaradny, H.: Simulation of Field Water Use and Crop Yield, Simulation Monographs, Centre for Agricultural Publishing and Documentation, Wageningen, 189 pp., 1978.
Fenicia, F., McDonnell, J. J., and Savenije, H. H. G.: Learning from model improvement: on the contribution of complementary data to process understanding, Water Resour. Res., 44, W06419, doi:10.1029/2007wr006386, 2008.
Fenicia, F., Wrede, S., Kavetski, D., Pfister, L., Hoffmann, L., Savenije, H. H. G., and McDonnell, J. J.: Assessing the impact of mixing assumptions on the estimation of streamwater mean residence time, Hydrol. Process., 24, 1730–1741, doi:10.1002/Hyp.7595, 2010.
Garvelmann, J., Külls, C., and Weiler, M.: A porewater-based stable isotope approach for the investigation of subsurface hydrological processes, Hydrol. Earth Syst. Sci., 16, 631–640, doi:10.5194/hess-16-631-2012, 2012.
Gazis, C. and Feng, X.: A stable isotope study of soil water: evidence for mixing and preferential flow paths, Geoderma, 119, 97–111, doi:10.1016/S0016-7061(03)00243-X, 2004.
Gehrels, J. C., Peeters, J. E., de Vries, J. J., and Dekkers, M.: The mechanism of soil water movement as inferred from O-18 stable isotope studies, Hydrolog. Sci. J., 43, 579–594, 1998.
Gribb, M. M., Forkutsa, I., Hansen, A., Chandler, D. G., and McNamara, J. P.: The effect of various soil hydraulic property estimates on soil moisture simulations, Vadose Zone J., 8, 321–331, doi:10.2136/vzj2008.0088, 2009.
Gupta, H., Beven, K., and Wagener, T.: Model calibration and uncertainty estimation, in: Encyclopedia of Hydrological Sciences, edited by: Anderson, M., John Wiley & Sons Ltd., Tucson, AZ, US, Lancaster, UK, 2006.

HESSD
11, 11203–11245, 2014

Hädrich, F. and Stahr, K.: Die Böden des Breisgaus und angrenzender Gebiete, Berichte der Naturforschenden Gesellschaft Freiburg i. Br., 143 pp., 2001.
Hartmann, A., Kralik, M., Humer, F., Lange, J., and Weiler, M.: Identification of a karst system's intrinsic hydrodynamic parameters: upscaling from single springs to the whole aquifer, Environ. Earth Sci., 65, 2377–2389, doi:10.1007/s12665-011-1033-9, 2012.
Hoffman, G. and van Genuchten, M.: Soil properties and efficient water use: water namagement for salinity control, in: Limitations and Efficient Water Use in Crop Production, edited by: Taylor, H., Jordan, W., and Sinclair, T., American Society Of Agrononmy, Madison, WI, 73–85, 1983.
Hopmans, J. W., Šimůnek, J., Romano, N., and Durner, W.: Inverse methods, in: Methods of Soil Analysis: Part 1 Physical Methods, Soil Science Society of America Book Series, vol. 5, 3rd Edn., edited by: Dane, J. H. and Topp, G. C., Soil Science Society of America, Madison, Wisconsin, USA, 963–1008, 2002.
Hornberger, G. M. and Spear, R. C.: An approach to the analysis of behavior and sensitivity in environmental systems, in: Uncertainty and Forecasting of Water Quality, edited by: Beck, M. and Straten, G., Springer, Berlin, Heidelberg, 101–116, 1983.
Imbery, F.: Langjährige Variabilität der aerodynamischen Oberflächenrauhigkeit und Energieflüsse eines Kiefernwaldes in der südlichen Oberrheinebene (Hartheim), Dissertation, Meteorologischen Instituts, Albert-Ludwigs-Universität Freiburg i. Br., Freiburg i. Br., 2005.
Inoue, M., Šimůnek, J., Shiozawa, S., and Hopmans, J. W.: Simultaneous estimation of soil hydraulic and solute transport parameters from transient infiltration experiments, Adv. Water Resour., 23, 677–688, 2000.
Jacques, D., Šimůnek, J., Timmerman, A., and Feyen, J.: Calibration of Richards' and convection–dispersion equations to field-scale water flow and solute transport under rainfall conditions, J. Hydrol., 259, 15–31, 2002.
Jaeger, L. and Kessler, A.: The HartX period May 1992, seen against the background of twenty years of energy balance climatology at the Hartheim pine plantation, Theor. Appl. Climatol., 53, 9–21, doi:10.1007/BF00866407, 1996.
Jarvis, N. J.: The MACRO model (Version 3.1), Technical Description and Sample Simulations, Reports and Dissertations 19, Dept. Soil Sci., Swedish Univ. Agric. Sci., Uppsala, Sweden, 1994.

HESSD
11, 11203–11245, 2014

Kling, H., Fuchs, M., and Paulin, M.: Runoff conditions in the upper Danube basin under an ensemble of climate change scenarios, J. Hydrol., 424–425, 264–277, doi:10.1016/j.jhydrol.2012.01.011, 2012.

Koeniger, P.: Tracerhydrologische Ansätze zur Bestimmung der Grundwasserneubildung, Dissertation, Institut für Hydrologie, Albert-Ludwigs-Universität Freiburg i. Br., Freiburg i. Br., 2003.

Koeniger, P., Leibundgut, C., Link, T., and Marshall, J. D.: Stable isotopes applied as water tracers in column and field studies, Stable Isotop. Biogeosci., 41, 31–40, doi:10.1016/j.orggeochem.2009.07.006, 2010.

Kool, J. B., Parker, J. C., and van Genuchten, M. T.: Determining soil hydraulic properties from one-step outflow experiments by parameter estimation: I. Theory and numerical studies, Soil Sci. Soc. Am. J., 49, 1348–1354, 1985.

Kuczera, G. and Mroczkowski, M.: Assessment of hydrologic parameter uncertainty and the worth of multiresponse data, Water Resour. Res., 34, 1481–1489, doi:10.1029/98WR00496, 1998.

Kumar, S., Sekhar, M., Reddy, D. V., and Mohan Kumar, M. S.: Estimation of soil hydraulic properties and their uncertainty: comparison between laboratory and field experiment, Hydrol. Process., 24, 3426–3435, 2010.

Kuntz, B. W., Rubin, S., Berkowitz, B., and Singha, K.: Quantifying solute transport at the Shale Hills critical zone observatory, Vadose Zone J., 10, 843–857, doi:10.2136/vzj2010.0130, 2011.

Lorz, C., Heller, K., and Kleber, A.: Stratification of the Regolith Continuum – a key property for processes and functions of landscapes, Z. Geomorphol. Supp., 55, 277–292, doi:10.1127/0372-8854/2011/0055S3-0062, 2011.

Maciejewski, S., Małoszewski, P., Stumpp, C., and Klotz, D.: Modelling of water flow through typical Bavarian soils: 1. Estimation of hydraulic characteristics of the unsaturated zone, Hydrolog. Sci. J., 51, 285–297, doi:10.1623/hysj.51.2.285, 2006.

Majoube, M.: Fractionnement en oxygene-18 et en deuterium entre l'eau et sa vapeur, J. Chim. Phys., 68, 1423–1436, 1971.

Maloszewski, P., Rauert, W., Stichler, W., and Herrmann, A.: Application of flow models in an alpine catchment area using tritium and deuterium data, J. Hydrol., 66, 319–330, doi:10.1016/0022-1694(83)90193-2, 1983.

HESSD
11, 11203–11245, 2014

Maloszewski, P., Rauert, W., Trimborn, P., Herrmann, A., and Rau, R.: Isotope hydrological study of mean transit times in an alpine basin (Wimbachtal, Germany), J. Hydrol., 140, 343–360, doi:10.1016/0022-1694(92)90247-S, 1992.

Maloszewski, P., Maciejewski, S., Stumpp, C., Stichler, W., Trimborn, P., and Klotz, D.: Modelling of water flow through typical Bavarian soils: 2. Environmental deuterium transport, Hydrolog. Sci. J., 51, 298–313, doi:10.1623/hysj.51.2.298, 2006.

Mayer, H., Schindler, D., Fernbach, G., and Redepenning, D.: Forstmeteorologische Messstelle Hartheim des Meteorologischen Institutes der Universität Freiburg, Meteorologisches Institut der Universität Freiburg, Freiburg i. Br., 2005.

McGuire, K. J. and McDonnell, J. J.: A review and evaluation of catchment transit time modeling, J. Hydrol., 330, 543–563, doi:10.1016/j.jhydrol.2006.04.020, 2006.

Medina, A., Carrera, J., and Galarza, G.: Inverse modelling of coupled flow and solute transport problems, in: ModelCARE 90: Calibration and Reliability in Groundwater Modelling, edited by: Kovar, K., September 1990, The Hague, IAHS-AISH Publ., 195, 185–194, 1990.

Mertens, J., Stenger, R., and Barkle, G. F.: Multiobjective inverse modeling for soil parameter estimation and model verification, Vadose Zone J., 5, 917–933, doi:10.2136/vzj2005.0117, 2006.

Millington, R. J. and Quirk, J. P.: Permeability of porous solids, T. Faraday Soc., 57, 1200, doi:10.1039/TF9615701200, 1961.

Mills, R.: Self-diffusion in normal and heavy water in the range 1–45.deg, J. Phys. Chem., 77, 685–688, doi:10.1021/j100624a025, 1973.

Mishra, S. and Parker, J. C.: Parameter estimation for coupled unsaturated flow and transport, Water Resour. Res., 25, 385–396, 1989.

Mualem, Y.: A new model for predicting the hydraulic conductivity of unsaturated porous media, Water Resour. Res., 12, 513–522, doi:10.1029/WR012i003p00513, 1976.

Pachepsky, Y., Benson, D., and Rawls, W.: Simulating scale-dependent solute transport in soils with the fractional advective–dispersive equation, Soil Sci. Soc. Am. J., 64, 1234–1243, 2000.

Pachepsky, Y., Smettem, K., Vanderborght, J., Herbst, M., Vereecken, H., and Wösten, J.: Reality and fiction of models and data in soil hydrology, in: Unsaturated-Zone Modeling: Progress, Challenges and Applications, edited by: Feddes, R. A., de Rooij, G. H., and van Dam, J. C., Springer, New York, 233–260, 2004.

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Pachepsky, Y., Rawls, W., and Lin, H.: Hydropedology and pedotransfer functions, Geoderma, 131, 308–316, doi:10.1016/j.geoderma.2005.03.012, 2006.
Perfect, E., Sukop, M. C., and Haszler, G. R.: Prediction of dispersivity for undisturbed soil columns from water retention parameters, Soil Sci. Soc. Am. J., 66, 696–701, doi:10.2136/sssaj2002.6960, 2002.
Pfister, L., Wagner, C., Vansuypeene, E., Drogue, G., and Hoffmann, L.: Atlas Climatique du Grand-Duché de Luxembourg, Musée National d'Histoire Naturelle, Bernkastel-Kues, 80 pp., 2005.
Revesz, K. and Woods, P. H.: A method to extract soil water for stable isotope analysis, J. Hydrol., 115, 397–406, doi:10.1016/0022-1694(90)90217-L, 1990.
Ritchie, J. T.: Model for predicting evaporation from a row crop with incomplete cover, Water Resour. Res., 8, 1204–1213, doi:10.1029/WR008i005p01204, 1972.
Ritter, A., Hupet, F., Muñoz-Carpena, R., Lambot, S., and Vanclooster, M.: Using inverse methods for estimating soil hydraulic properties from field data as an alternative to direct methods, Agr. Water Manage., 59, 77–96, 2003.
Roa-García, M. C. and Weiler, M.: Integrated response and transit time distributions of watersheds by combining hydrograph separation and long-term transit time modeling, Hydrol. Earth Syst. Sci., 14, 1537–1549, doi:10.5194/hess-14-1537-2010, 2010.
Russo, D., Bresler, E., Shani, U., and Parker, J. C.: Analyses of infiltration events in relation to determining soil hydraulic properties by inverse problem methodology, Water Resour. Res., 27, 1361–1373, doi:10.1029/90WR02776, 1991.
Schaap, M. G., Leij, F. J., and van Genuchten, M. T.: ROSETTA: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions, J. Hydrol., 251, 163–176, doi:10.1016/S0022-1694(01)00466-8, 2001.
Schäfer, G.: Nährelementehaushalt von Kiefernjungbeständen in der südlichen Oberrheinebene, Freiburger Bodenkundliche Abhandlungen, Freiburg, 153 pp., 1977.
Šimůnek, J., Sejna, M., Saito, H., Sakai, M., and van Genuchten, M. T.: The HYDRUS-1D Software Package for Simulating the One-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media, Version 4.15, Riverside, California, 2012.
Spear, R. C. and Hornberger, G. M.: Eutrophication in peel inlet – II. Identification of critical uncertainties via generalized sensitivity analysis, Water Res., 14, 43–49, doi:10.1016/0043-1354(80)90040-8, 1980.

HESSD
11, 11203–11245, 2014

Strasser, U. and Mauser, W.: Modelling the spatial and temporal variations of the water balance for the Weser catchment 1965–1994, J. Hydrol., 254, 199–214, doi:10.1016/S0022-1694(01)00492-9, 2001.

Stumpp, C., Maloszewski, P., Stichler, W., and Fank, J.: Environmental isotope (δ^{18}O) and hydrological data to assess water flow in unsaturated soils planted with different crops: case study lysimeter station "Wagna" (Austria), J. Hydrol., 369, 198–208, doi:10.1016/j.jhydrol.2009.02.047, 2009a.

Stumpp, C., Stichler, W., and Maloszewski, P.: Application of the environmental isotope δ^{18}O to study water flow in unsaturated soils planted with different crops: case study of a weighable lysimeter from the research field in Neuherberg, Germany, J. Hydrol., 368, 68–78, doi:10.1016/j.jhydrol.2009.01.027, 2009b.

Stumpp, C., Stichler, W., Kandolf, M., and Šimůnek, J.: Effects of land cover and fertilization method on water flow and solute transport in five lysimeters: a long-term study using stable water isotopes, Vadose Zone J., 11, vzj2011.0075, doi:10.2136/vzj2011.0075, 2012.

Thomas, E. M., Lin, H., Duffy, C. J., Sullivan, P. L., Holmes, G. H., Brantley, S. L., and Jin, L.: Spatiotemporal patterns of water stable isotope compositions at the Shale Hills critical zone observatory: linkages to subsurface hydrologic processes, Vadose Zone J., 12, vzj2013.01.0029, doi:10.2136/vzj2013.01.0029, 2013.

Vanclooster, M., Boesten, J., Tiktak, A., Jarvis, N., Kroes, J., Muñoz-Carpena, R., Clothier, B., and Green, S.: On the use of unsaturated flow and transport models in nutrient and pesticide management, in: Unsaturated-Zone Modeling: Progress, Challenges and Applications, edited by: Feddes, R. A., de Rooij, G. H., and van Dam, J. C., 6, Springer, New York, 331–361, 2004.

Vanderborght, J. and Vereecken, H.: Review of dispersivities for transport modeling in soils, Vadose Zone J., 6, 29–52, doi:10.2136/vzj2006.0096, 2007.

van Genuchten, M. T.: A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sci. Soc. Am. J., 44, 892–898, 1980.

Vereecken, H., Weynants, M., Javaux, M., Pachepsky, Y., Schaap, M. G., and van Genuchten, M.: Using pedotransfer functions to estimate the van Genuchten–Mualem soil hydraulic properties: a review, Vadose Zone J., 9, 795–820, doi:10.2136/vzj2010.0045, 2010.

Vrugt, J. A. and Bouten, W.: Validity of first-order approximations to describe parameter uncertainty in soil hydrologic models, Soil Sci. Soc. Am. J., 66, 1740, doi:10.2136/sssaj2002.1740, 2002.

HESSD
11, 11203–11245, 2014

Vrugt, J. A., Stauffer, P. H., Wöhling, T., Robinson, B. A., and Vesselinov, V. V.: Inverse modeling of subsurface flow and transport properties: a review with new developments, Vadose Zone J., 7, 843–864, doi:10.2136/vzj2007.0078, 2008.

Wassenaar, L., Hendry, M., Chostner, V., and Lis, G.: High resolution pore water δ^2H and δ^{18}O Measurements by H_2O (liquid)–H_2O (vapor) equilibration laser spectroscopy, Environ. Sci. Technol., 42, 9262–9267, doi:10.1021/es802065s, 2008.

Wellings, S.: Recharge of the Upper Chalk aquifer at a site in Hampshire, England: 2. Solute movement, J. Hydrol., 69, 275–285, doi:10.1016/0022-1694(84)90167-7, 1984.

Wenzel, A., Kalthoff, N., and Fiedler, F.: On the variation of the energy-balance components with orography in the Upper Rhine Valley, Theor. Appl. Climatol., 57, 1–9, doi:10.1007/BF00867973, 1997.

Wesseling, J. G.: Meerjarige Simulaties van Gronwateronttrekking voor Verschillende Bodmprofielen, Grondwatertrappen en Gewassen met het Model SWATRE, Report 152, Winand Staring Centre, Wageningen, Netherlands, 1991.

Whisler, F. D. and Watson, K. K.: One-dimensional gravity drainage of uniform columns of porous materials, J. Hydrol., 6, 277–296, 1968.

Wöhling, T., Vrugt, J. A., and Barkle, G. F.: Comparison of three multiobjective optimization algorithms for inverse modeling of vadose zone hydraulic properties, Soil Sci. Soc. Am. J., 72, 305–319, doi:10.2136/sssaj2007.0176, 2008.

Zhang, Z. F., Ward, A. L., and Gee, G. W.: Estimating soil hydraulic parameters of a field drainage experiment using inverse techniques, Vadose Zone J., 2, 201–211, doi:10.2113/2.2.201, 2003.

Zimmermann, U., Münnich, K. O., Roether, W., Kreutz, W., Schubach, K., and Siegel, O.: Tracers determine movement of soil moisture and evapotranspiration, Science, 152, 346–347, doi:10.1126/science.152.3720.346, 1966.

Zimmermann, U., Ehhalt, D., and Münnich, K.: Soil-water movement and evapotranspiration: changes in the isotopic composition of the water, in: Isotopes in Hydrology, IAEA, Isotopes in Hydrology, 14–18 November 1966, Vienna, International Atomic Energy Agency, Vienna, 567–585, 1967.

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Table 1. Environmental characteristics of the three study sites and the available data for the fitting targets for the inverse modelling.

		Roodt	Eichstetten	Hartheim
Location		49°82′ N; 5°83′ E	48°05′ N; 7°42′ E	47°56′ N; 7°36′ E
Elevation m a.s.l.		470 m	310 m	200 m
Geology		Devonian Schist[a]	Pleistocene aeolian loess	Fluvial Gravel[d]
Soil type		Cambisol	Luvisol	Calcaric Regosol[d]
Soil depth	Horizon 1	0–25 cm	0–25 cm	0–40 cm[d]
	Horizon 2	> 25 cm	> 25 cm	> 40 cm[d]
Soil texture	Horizon 1	loam	slightly clayey silt	Silty sand[d]
	Horizon 2	clayey loam	slightly clayey silt	fluvial gravel and coarse sand[d]
Mean annual temperature [°C]		8.3[b]	11	9.8[e]
Mean annual precipitation [mm]		845[b]	900	667[e]
Land use		Grassland	Grassland	*Pinus sylvestris* (Scots pine)[e]
Soil moisture data	Sampling period	Daily (22 Mar 2013–15 Mar 2014)	Daily (31 Jul 2012–31 May 2013)	Biweekly (29 Apr 1998–13 Jan 2000)
	Sampling depth [cm]	−10, −30, −50	−5, −10, −20, −30, −40, −50, −60	−2, −10,-30
	Sampling method	5TE sensors (Decagon)	5TE sensors (Decagon)	Gravimetric with soil cores[f]
Isotope profiles sampling		2	3	16
Pore water isotope analysis		Equilibrium method[c]	Equilibrium method[c]	azeotropic distillation with toluol and mass spectrometer[g]
Model period		1 Jan 2008–31 Dec 2013	1 Jan 2008–4 Nov 2013	1 Jan 1997–31 Dec 2002

[a] Lorz et al. (2011); [b] Pfister et al. (2005); [c] Wassenaar et al. (2008); [d] Schäfer (1977); [e] Mayer et al. (2005); [f] Koeniger (2003); [g] Revesz and Woods (1990).

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Table 2. Boundaries of the parameter space for the unconstrained inverse model approaches (uIPA, MOA, 2SA).

Parameter	Lower boundary	Upper boundary
Residual volumetric water content, θ_r [$cm^3\,cm^{-3}$]	0	0.2
Saturated volumetric water content, θ_s [$cm^3\,cm^{-3}$]	0.2	0.7
inverse of the capillary fringe thickness, α [cm^{-1}]	0.001	0.1
MVG shape parameter, n [–]	1.1	2.5
Saturated hydraulic conductivity, K_s [$cm\,d^{-1}$]	10	400
Longitudinal dispersivity, λ [cm]	0	30

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Table 3. Performance of the different inverse model approaches regarding the soil moisture (KGE_θ) and isotope (KGE_D) data and the average of this both efficiency measure (KGE_{tot}) for the three study sites. (Perfect fit would result in a Kling–Gupta-Efficiency (KGE) of 1.)

	Roodt			Eichstetten			Hartheim		
	KGE_θ	KGE_D	KGE_{tot}	KGE_θ	KGE_D	KGE_{tot}	KGE_θ	KGE_D	KGE_{tot}
uIPA	−0.35	0.83	0.24	0.37	0.86	0,31	0.10	0.72	0.41
IPA	−0.15	0.72	0.28	0.37	0.80	0.58	0.24	0.65	0.45
MOA	0.70	0.69	0.70	0.79	0.82	0.80	0.20	0.67	0.44
2SA	0.80	0.62	0.71	0.80	0.79	0.80	0.43	0.40	0.41

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Table 4. Best performing parameter sets of the different optimization approaches for the three different study sites.

Study site	Optimization approach	Horizon	θ_r	θ_s	α	n	K_s	λ
Roodt	uIPA	1	0.065	0.358	0.089	2.10	295	4.3
		2	0.072	0.434	0.017	1.13	238	1.0
	IPA	1	0.044	0.384*	0.027*	1.66*	24	23.2
		2	0.074	0.384*	0.008*	1.52*	15*	0.4
	MOA	1	0.115	0.312	0.081	1.23	378	2.7
		2	0.014	0.244	0.047	1.17	301	1.0
	2SA	1	0.052	0.254	0.001	1.30	242	9.0
		2	0.021	0.225	0.007	1.14	242	0.1
Eichstetten	uIPA	1	0.197	0.214	0.040	2.07	355	7.1
		2	0.026	0.668	0.001	1.21	129	4.2
	IPA	1	0.038	0.488*	0.007*	1.48*	40	0.1
		2	0.067	0.476	0.008	1.54	14	2.5
	MOA	1	0.122	0.601	0.003	1.59	76	0.7
		2	0.012	0.609	0.005	1.38	394	1.8
	2SA	1	0.076	0.654	0.007	1.42	185	0.5
		2	0.011	0.585	0.005	1.39	306	1.8
Hartheim	uIPA	1	0.179	0.367	0.026	1.90	237	8.0
		2	0.045	0.280	0.095	2.21	243	0.0
	IPA	1	0.059	0.387*	0.011	1.35	104*	8.2
		2	0.041	0.388	0.026*	1.45	104*	0.2
	MOA	1	0.141	0.292	0.006	1.83	308	9.1
		2	0.028	0.219	0.052	2.06	228	15.2
	2SA	1	0.004	0.522	0.078	1.22	6	1.8
		2	0.104	0.636	0.036	2.17	223	29.2

* indicate parameters that reached the initial boundaries of the parameter space in the IPA.

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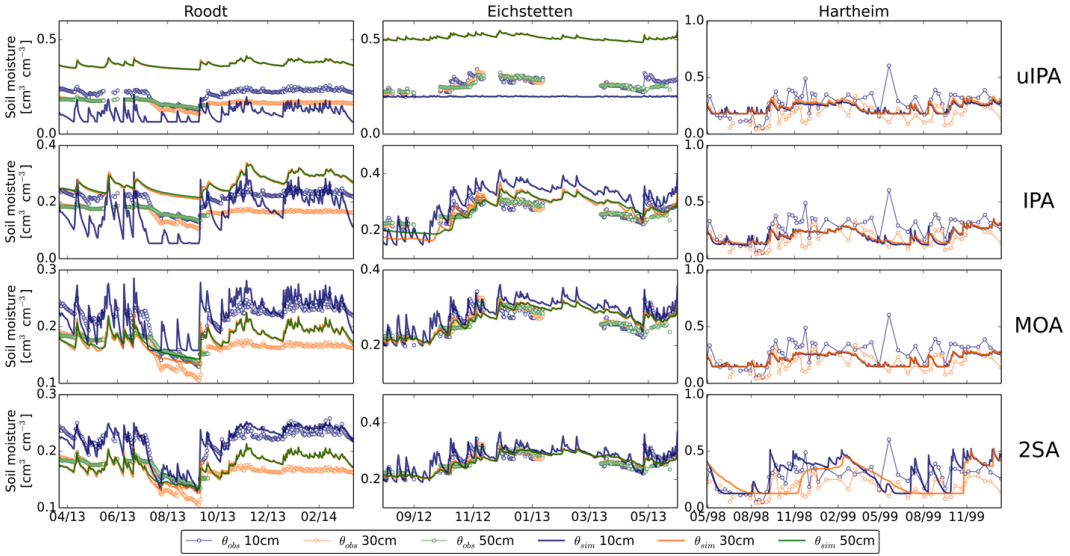

Figure 1. Observed soil moisture (circles) at each study site and the corresponding simulated soil moisture (lines), modelled with the best parameter set derived from the three different inverse model approaches. Two or three observed soil moisture time series are shown. uIPA: unconstrained isotope profile approach; IPA: isotope profile approach; MOA: multi-objective approach; 2SA: two-step approach.

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Estimating flow and transport parameters in the unsaturated zone with pore water stable isotopes

M. Sprenger et al.

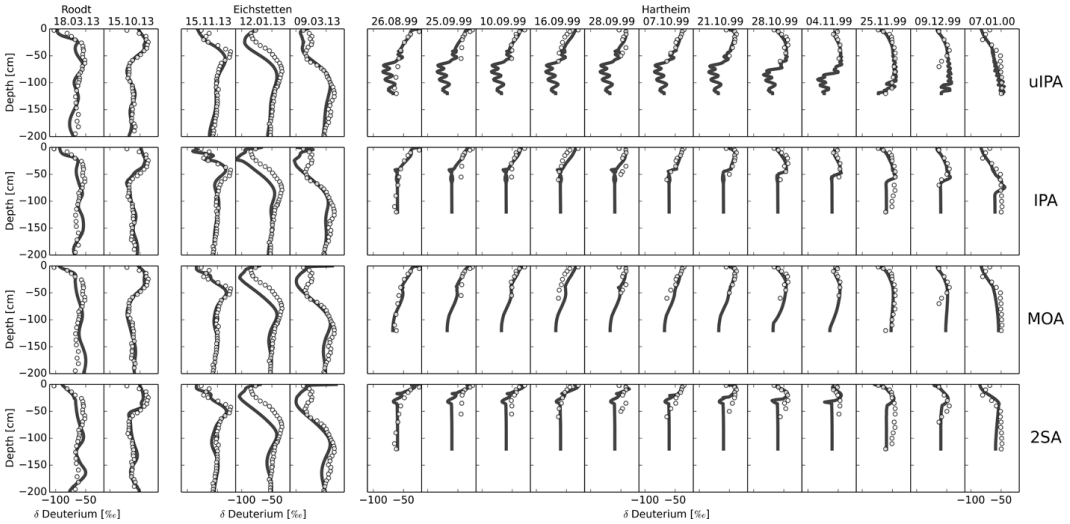

Figure 2. Observed (circles) and simulated (lines) pore water deuterium concentrations at each study site and at various dates. Simulations done with the best parameter set derived from the three different inverse model approaches. Axes scaling kept constant for each subplot.

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Figure 3. Parameter identifiability of each parameter calibrated at each site with the different inverse model approaches (uIPA, IPA, MOA, 2SA) for the upper (1) and lower (2) soil horizon. Colour indicates the normalized parameter ranges between the 10th and the 90th percentile of the 10 % best optimization runs as a percentage of the initial boundaries of the parameter space.

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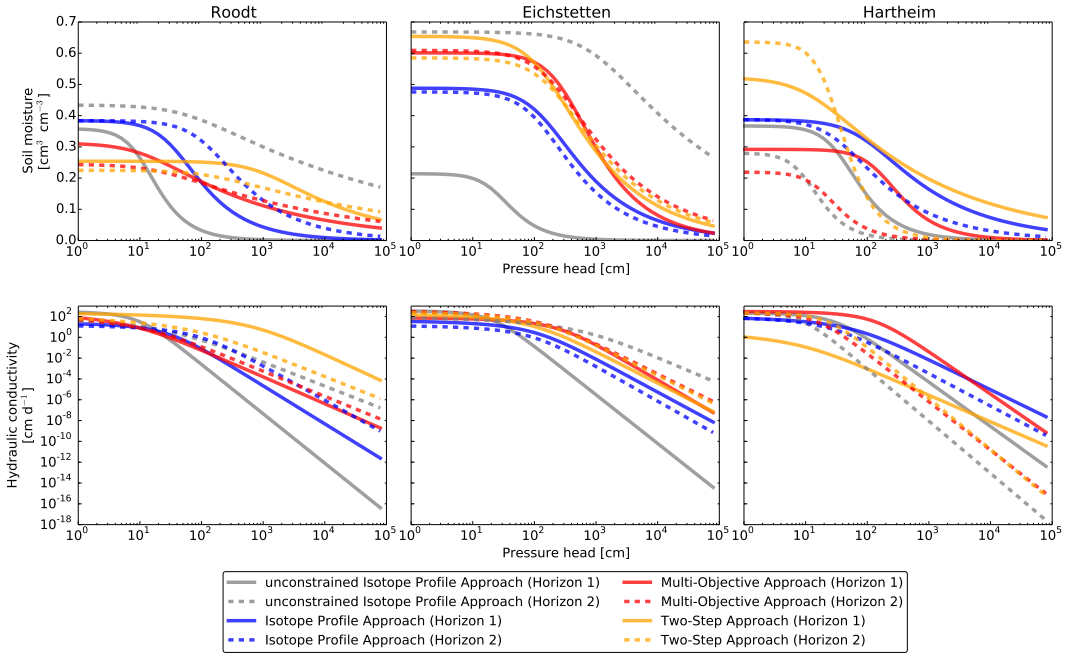

Figure 4. The water retention and the hydraulic conductivity functions for the parameter sets of the upper and lower soil horizons (continuous and dashed line, respectively), that resulted in the best model performance after calibrating with the three different inverse modelling approaches for each study site. Note that with respect to these characteristic curves the 3 calibration approaches are based on only isotope data (uIPA), a mix of isotope data and soil texture data (IPA), a mix of isotope and soil moisture data (MOA) and only soil moisture data (2SA).

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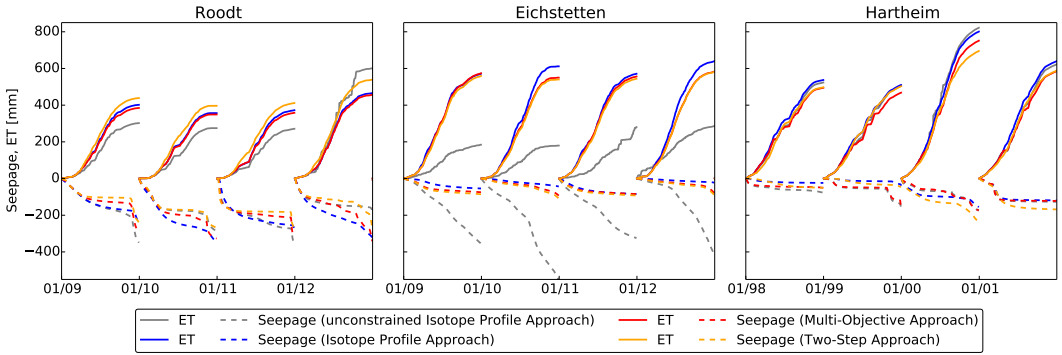

Figure 5. Annual cumulative seepage (dashed lines) and actual evapotranspiration (continuous lines) simulated with the best parameter sets optimized with the different inverse modelling approaches for each site.

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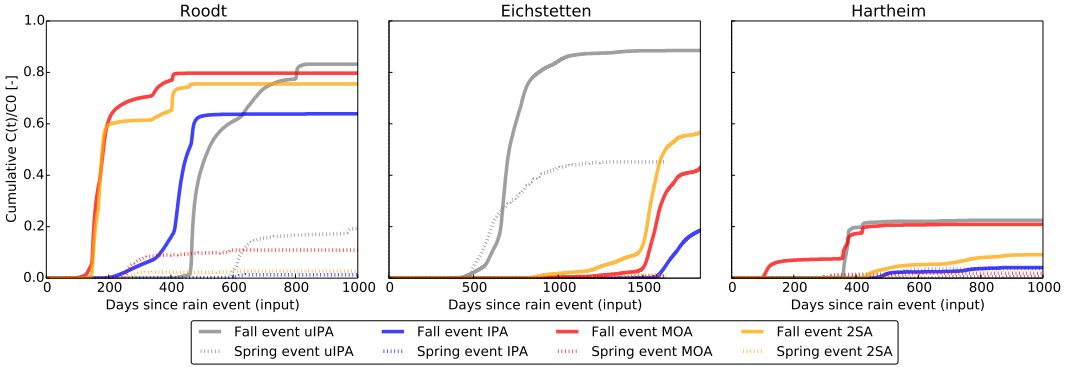

Figure 6. Cumulative transit time distribution of rainwater infiltrated during an event in fall (continuous line) and spring (dotted line) in the seepage flux. Simulations were done with the parameter sets that performed best during the different inverse modelling approaches (colours) at each study site.

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