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Nested-scale discharge and groundwater level monitoring to improve predictions of flow route discharges and nitrate loads

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Identifying effective measures to reduce nutrient loads of headwaters in lowland catchments requires a thorough understanding of flow routes of water and nutrients. In this paper we assess the value of nested-scale discharge and groundwater level measurements for predictions of catchment-scale discharge and nitrate loads. In order to relate field-site measurements to the catchment-scale an upscaling approach is introduced that assumes that scale differences in flow route fluxes originate from differences in the relationship between groundwater storage and the spatial structure of the groundwater table. This relationship is characterized by the Groundwater Depth Distribution (GDD) curve that relates spatial variation in groundwater depths to the average groundwater depth. The GDD-curve was measured for a single field site (0.009 km²) and simple process descriptions were applied to relate the groundwater levels to flow route discharges. This parsimonious model could accurately describe observed storage, tube drain discharge, overland flow and groundwater flow simultaneously with Nash-Sutcliff coefficients exceeding 0.8. A probabilistic Monte Carlo approach was applied to up-scale field-site measurements to catchment scales by inferring scale-specific GDD-curves from hydrographs of two nested catchments (0.4 and 6.5 km²). The estimated contribution of tube drain effluent (a dominant source for nitrates) decreased with increasing scale from 76–79% at the field-site to 34–61% and 25–50% for both catchment scales. These results were validated by demonstrating that a model conditioned on nested-scale measurements simulates better nitrate loads and better predictions of extreme discharges during validation periods compared to a model that was conditioned on catchment discharge only.

1 Introduction

Intensive agriculture in lowland catchments often leads to high nitrate losses and eutrophication of downstream waters (Oenema, 2007; Van der Molen, 1998; Vitousek

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et al., 2009). To identify effective measures to reduce these nitrate loads, the flow routes of water that enter a stream and their nutrient concentrations need to be quantified (Tiemeyer et al., 2010). In densely drained lowland catchments, surface water discharge is fed by groundwater flow toward streams and ditches, tile drain effluent, and overland flow. Many field-scale studies identified tube drain effluent as the major source of nitrate (Tiemeyer et al., 2006; Nangia et al., 2010; Rozemeijer et al., 2010c). However, the field scale at which these contributions can be directly measured (De Vos et al., 2000; Van der Velde et al., 2010a) often is not the scale of interest to water management authorities. Extrapolation of fields site results to entire catchments can easily lead to wrong conclusions as field sites can prove non-representative of the patterns and processes that emerge at larger scales (Sivapalan, 2003; Soulsby et al., 2006; Didszun and Uhlenbrook, 2008). Therefore, our challenge is to effectively integrate information from field-scale measurements into the prediction of catchment-scale flow route contributions.

In Van der Velde et al. (2010a), we presented the results of a field-scale measurement setup that separated tile drain flow from overland flow and groundwater flow. We also measured discharges at two larger nested scales and showed that, rather than the actual measured volumes at the field site, the characteristic response of individual flow routes can be used to upscale the field-site flow routes to the catchment scale. This elementary upscaling approach was purely based on measured data. A model framework was needed to upscale the measured field-scale fluxes to catchment-scale contributions of flow routes for periods without complete sets of measurements.

To develop such a model upscaling approach, Sivapalan (2003) advocated the search for concepts that “easily connect scales, and that can also be easily scaled”. This should lead to “a watershed-scale representation that is clearly tied to process descriptions at a lower level of scale, and which is not overly complex”. In sloped terrain, scaling research has focused on the way in which hillslopes connect to headwaters (Uchida et al., 2005; Jensco et al., 2009; Tetzlaff et al., 2008; Clark et al., 2009) and headwaters to entire basins (Shaman et al., 2004). Rodgers et al. (2005),

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Tetzlaff et al. (2007), and Didszun and Uhlenbrook (2008) studied the scaling behavior of both discharge and tracers across nested-scale catchments and found that scaling effects in discharge and solutes could largely be attributed to scale-related morphologic, topographic and land-use features. In contrast to sloped catchments, lowland catchments generally have little morphological heterogeneity and the main flow routes occur at all scales. Therefore, the scale effects in discharge of lowland catchments are primarily driven by scale-differences in drainage density of ditches and tube drains, micro-topography, and soil type.

In Van der Velde et al. (2009) we proposed an upscaling approach for hydrology in lowland catchments (from here on called the Lowland Groundwater-Surface water Interaction model, LGSI-model). We assumed there that each flow route (i.e., ditch and stream drainage, overland flow, and tube drain flow) starts to discharge if the groundwater level exceeds a flow route-specific threshold groundwater level at that location, and that the magnitude of the flux depends on the groundwater level. The contribution of a flow route to the total catchment discharge is calculated by integration over all groundwater levels in the catchment, described by a groundwater depth distribution. Van der Velde et al. (2009) showed that each storage volume of groundwater in the saturated zone corresponds to a unique groundwater depth distribution. They also showed that the relation between storage and groundwater depth distribution can be defined at any spatial scale and has the same basic shape at any scale and thus satisfies Sivapalan's (2003) criterion: it "easily connects scales, and can also be easily scaled".

However, in order to measure this relationship between storage and the groundwater depth distribution at catchment scales relevant to water management authorities, many groundwater depth time series are needed throughout the catchment. This makes this approach laborious and in our previous paper (Van der Velde et al., 2009) we had to resort to spatially distributed transient groundwater modeling to derive this relationship. A workable alternative would be to have a dense network of groundwater monitoring wells on a small area within the catchment, and observe the groundwater levels

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frequently for a limited time period. Obviously some sort of upscaling is then needed to use this data to characterize the behavior of the entire catchment. We introduce here a nested-scale model setup combined with a probabilistic Monte Carlo approach to achieve this.

5 The objectives of this paper are twofold. Firstly, we test whether the LGSI-model can accurately describe all individual flow route fluxes at the field scale. This would increase our confidence in the ability of the LGSI-model to simulate flow route fluxes accurately at the catchment scale where these fluxes cannot be measured directly. Secondly, we want to assess the value of nested-scale monitoring as presented in Van
10 der Velde et al. (2010a) for reducing uncertainty in predictions of catchment-scale flow route discharges.

2 Materials and methods

This paper combines the nested-scale measurements introduced by Van der Velde et al. (2010a) and the upscaling approach described in Van der Velde et al. (2009). Therefore, we offer a brief summary of the relevant information (Sects. 2.1 and 2.2), and refer
15 to both papers for detailed background information. The LGSI-model is first applied to the field-site discharge and groundwater level measurements, which are described in Sect. 2.3. Section 2.4 introduces a catchment model conditioned on catchment discharge and a groundwater level time series and in Sect. 2.5 the field-site model and
20 the catchment model are combined into a nested-scales model. Section 2.6 introduces validation strategies for both the catchment model and the nested-scales model to assess the value of nested scale monitoring.

2.1 Nested experimental setup

25 The measurements for this study were performed in the Hupsel Brook catchment in the eastern part of The Netherlands (Fig. 1a) (52°06' N; 6°65' E). The size of the catchment

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is 6.5 km², with surface elevations ranging from 22 to 36 m a.s.l. (above sea level). At depths ranging from 0.5 to 20 m an impermeable marine clay layer is found (Van Ommen et al., 1989). The unconfined aquifer consists of Pleistocene aeolian sands with occasional layers of clay, peat, and gravel (see Wösten et al., 1985, for more details).

The Hupsel Brook catchment is drained by a straightened and deepened main brook and by a dense artificial drainage network of ditches and tube drains. The spacing between the ditches averages 300 m (Fig. 1a) and approximately 50% of the area has tube drains (plastic perforated flexible tubes). The Hupsel Brook catchment has a semi-humid sea climate with a yearly precipitation of 500 to 1100 mm and a yearly estimated evaporation of 300 to 600 mm, resulting in an estimated recharge of 200 to 800 mm per year.

Within the Hupsel Brook catchment, discharge was measured at three nested spatial scales: (1) the entire catchment of approximately 6.5 km², (2) a sub-catchment of 0.4 km² and (3) a 0.009 km² field site located within the sub-catchment (Fig. 1b). From August 2007 through December 2008, discharge was measured every 15 min for both catchment scales. Continuous surface water nitrate concentrations were measured at the outlet of the entire catchment with a Hydrion-10 multi-parameter probe (Hydrion BV Wageningen, The Netherlands). Monthly average nitrate concentrations of tube drain effluent were measured at 20 locations in the catchment with Sorbi-Samplers (Roze-meijer et al., 2010a).

The tube drained field site of 0.9 ha had a drain spacing of 14.5 m. Along a 43.5 m stretch inside the deep easterly ditch (Fig. 1c), we built in-stream reservoirs with separate vessels to capture tube drain discharge. The in-stream reservoirs collected overland flow and groundwater influx through the stream bed. Thus we separated the tube drain flow from the combined flux of overland flow and groundwater flow. The discharge of both flow routes was measured with 5 min intervals for November 2007 through December 2008. During that period we also manually measured phreatic groundwater levels at 31 locations within the field-site every week. Pressure sensors

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in 15 piezometers along drain 1 (Fig. 1c) recorded phreatic levels every 10 min. A meteorological station of the KNMI (Royal Dutch Meteorological Institute) bordering the field-site measured hourly rainfall and evapotranspiration derived with the Makkink relation (Makkink, 1957).

2.2 Lowland groundwater-surface water interaction (LGSi) model

2.2.1 Basic model equations

The LGSi-model (Van der Velde et al., 2009) essentially consists of point-scale expressions of flow route fluxes (tube drain flow, overland flow, groundwater flow, direct rainfall, and evapotranspiration) and storages (saturated storage, unsaturated storage, and surface storage). A point in the catchment starts to generate a flux for a certain flow route when its groundwater level exceeds a threshold specific to that flow route. The magnitude of this flux (except for evapotranspiration) is directly proportional to the difference between the groundwater level and the threshold level. Upscaling of fluxes and storages is achieved by integrating the point-scale expressions over all groundwater depths within a model area. This distribution of groundwater depths was found to approximate a normal distribution with a mean and standard deviation that are a unique function of the total water storage. We formalized this function by the Groundwater Depth Distribution curve (GDD-curve) that describes the relationship between the spatial average groundwater depth and the spatial groundwater depth standard deviation.

The model parameters can be subdivided into process-specific parameters that describe fluxes and storages as a function of the local groundwater level and scale-specific parameters that describe the spatial distribution of groundwater depths, the total catchment area, the tube-drained area, and the area occupied by the surface water network. In Table 1 all point-scale process formulations, the GDD-curve, and their parameters are introduced. The complete set of LGSi-model equations is summarized in Appendix B. The LGSi-model is a fast calculating process model that calculates flow

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route discharges for a decade on hourly basis within a few seconds. This is a huge advantage over fully distributed models (e.g. Rozemeijer et al., 2010b), and allows for extensive parameter estimation by Monte Carlo simulation as will be demonstrated in this paper. However, the model is less suited to evaluate the effects of measures that affect the shape of the groundwater table, since this shape is derived from measurements and not calculated from physical principles.

2.2.2 Model extensions for the field site

To apply the LGSI-model to the field site, the basic setup needed to be extended to explicitly include groundwater flow out of the field into the deep ditch, lateral groundwater flow into the field from adjacent fields, and a time-variant flow resistance of the tube drains.

The single deep ditch to the east of the field is an anomaly in the surface elevation and is not well represented by the assumption of a normal distribution of groundwater depths (at larger scales with many different drainage depths a normal distribution is more appropriate). To account for groundwater flow towards this ditch, we introduce a new discharge term that approximates the groundwater flux to the deep ditch as a function of the average groundwater depth in the field, $\langle u(t) \rangle$ [L]:

$$Q_{\text{grw,field}}(t) = \frac{u_{\text{ditch}} - \langle u(t) \rangle}{r_{\text{ditch}}} \text{ for } u_{\text{ditch}} > \langle u(t) \rangle \quad (1)$$

with u_{ditch} [L] the depth of the ditch relative to the mean surface elevation of the field site area and r_{ditch} [T], the resistance of the field-site to groundwater flow towards the ditch. The lateral groundwater inflow, L_f [L T⁻¹], was assumed constant throughout the simulation period.

The total discharge measured by the in-stream reservoirs of the field experiment, Q_{res} [L T⁻¹], can now be calculated by all the water that enters the surface water except for the tube drain flux:

$$Q_{\text{res}}(t) = Q_{\text{grw,field}}(t) + Q_{\text{ov}}(t) + P_{\text{Q}}(t) - E_{\text{Q}}(t) \quad (2)$$

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with Q_{ov} the flux by overland flow, P_Q rainfall on ponded surfaces (including the ditch) and E_Q evaporation from ponded surfaces (all $L T^{-1}$).

During the experimental period, we observed a strong decline in the drainage effectiveness of the tube drains. At the beginning of the experiment the tube drains were cleaned by pressure flushing as is common practice in the Hupsel Brook catchment. This pressure flushing is repeated every two years. We hypothesized that the tube drains slowly get clogged in periods with substantial discharge and that in dry periods without discharge, aeration and oxidation of the clogging material inside the tube drains reduces the resistance. Similar behavior was also observed by Bentley and Skaggs (1993). The following simple empirical relation was adopted to account for the tube drain resistance change as a function of cumulative discharge:

$$\frac{dr_{dr}}{dt} = 1_{\{Q_{dr} > c_{dr}\}} a_{dr} - 1_{\{Q_{dr} < c_{dr}\}} b_{dr} r_{dr} \quad (3)$$

with a_{dr} [-] the rate with which the drainage resistance, r_{dr} [T], increases when the tube drain discharge is larger than threshold discharge c_{dr} [$L^3 T^{-1}$]. The resistance decreases with fractional rate b_{dr} [T^{-1}] for discharges smaller than c_{dr} .

2.2.3 Probabilistic parameter estimation

A parsimonious process model as the LGSI-model necessarily suffers from equifinality (parameter non-uniqueness; Beven and Freer, 2001) stemming from parameter uncertainty, the lumped nature of the parameters, the subjectivity introduced by including and excluding processes, the chosen process formulations, and the many different types of measurements that the model needs to describe. We dealt with equifinality by generating many combinations of parameters in a Monte Carlo procedure (GLUE methodology; Beven and Freer, 2001).

In this study we introduce three LGSI-models: a field-site model, a catchment model, and a nested-scales model. For each model, random parameter values were generated from prior uniform and independent distributions between predetermined parameter

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5 ranges. All parameter ranges are listed in Table 2 and were determined from literature data, field observations, topographic maps, and surface elevation maps. Parameter sets were qualified behavioral when the model satisfactory described the measured data and all behavioral parameter sets were considered equally probable. The criteria that divide the parameter space in behavioral and non-behavioral parameter sets are listed in Table 3, which will be further explained in the next three sections. This procedure was continued for each model until an ensemble of 500 behavioral parameter sets was found. This Monte Carlo multi-criteria model conditioning procedure is a simple but partly subjective and computationally inefficient procedure to generate ensembles of parameter sets. Many (mostly more complicated) variations of this procedure are possible and the subjectivity of the criteria that divide parameter sets in behavioral and non-behavioral may influence the uncertainty in model results. However, the proposed procedure is deemed accurate enough for the objectives of this study: to model field-site flow routes and to assess the value of nested-scale discharge and groundwater level monitoring for discharge and nitrate load predictions.

2.3 Field-site model of flow route fluxes

2.3.1 Interpretation of field site data

20 The field-site groundwater level measurements were converted to field-site average groundwater depths, standard deviations of groundwater depths, and volumes of ponds on the soils surface to comply with the variables of the LGSI-model. The measured absolute groundwater levels at 31 locations within the field (Fig. 1c) were interpolated to arrive at a groundwater table for the entire field (essentially, the interpolation weights the individual measured groundwater depths with their representative area). Subsequently, this groundwater table was subtracted from a detailed DEM (5 × 5 m resolution) and all groundwater depths were grouped into a groundwater depth distribution. The volume of negative groundwater depths of this distribution quantifies the volume of ponds on the field. A mean and standard deviation of the groundwater

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depth distribution and the volume of ponds were calculated for all 57 weekly field-site groundwater depth surveys. Continuous groundwater level measurements in the 15 groundwater wells around the tube drain 1 (Fig. 1c) were used to interpolate between the weekly field average groundwater depths in order to create a continuous field average groundwater depth time series.

2.3.2 Parameter estimation of field-site LGSI-model

The field-site model is conditioned on 5 sources of measured data:

- The measured relation between the average groundwater depth and the standards deviation of groundwater depth (GDD-data),
- The measured relation between the average groundwater depth and the volume of surface storage (Ponding-data),
- Time series of the spatial average groundwater depth,
- Time series of tube drain discharge,
- Time series of discharge measured by the in-stream reservoirs.

Figure 2 shows the five sequential steps that were followed to generate an ensemble of Behavioral Parameter Sets (BPS-FS). The specific order of these steps is determined by the relation between model equations and measured data. In the first step, the parameters for the GDD-curve (Eq. B7) are conditioned on the measured GDD-data. Secondly, the single parameter of the ponding-curve (Eq. B4), which also depends on the GDD-curve, is conditioned on the measured ponding-data. In the third step, storage (Eqs. B1–B3, B5, and B6), which depends on both the GDD-curve and the ponding-curve, is conditioned on the observed time series of the average groundwater depth. The measured tube drain and reservoir fluxes were used as input variables, which allowed the storage parameters to be estimated independently from the flux parameters.

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In the fourth step, the flow route fluxes (Eqs. B9 and B10) were conditioned on the measured tube drain and reservoir fluxes. The measured average groundwater depth was an input variable and hence was not calculated by the model. In the last step, a complete LGSI-model run allowed to check if the combination of the parameters still yielded an accurate model. These 5 steps were repeated until 500 behavioral parameter sets (BPS-FS) were found. The parameter distributions of BPS-FS were analyzed to determine parameter sensitivity and the model results were analyzed to quantify the uncertainty in flow route contributions to the total discharge owing to equifinality.

2.4 Catchment model

The parameters of the catchment model were conditioned on catchment discharge and a single groundwater level time series. The resulting ensemble of Behavioral Parameter Sets is referred to by BPS-C. Table 2 lists the parameter ranges from which the parameter sets were generated. The ranges for the process-specific parameters were equal to those used for the field-site model. Only the ranges for the scale-specific parameters that described areas (i.e. the catchment area, the tube drained area, and the area of the surface water network), which could be estimated from maps, were different.

The single groundwater level time series was not considered representative for the dynamics of the groundwater storage of the entire catchment. From field experience, we estimated that at any one time, at least 10% of the catchment area had shallower groundwater and another 10% had deeper groundwater than the single observed level: the observed groundwater level thus was assumed to be within the 0.10 and 0.90 percentile but allowing for an average exceedence of 1.0 cm (*GE*, Table 3).

2.5 Nested-scales model setup

We attempted to constrain the uncertainty in flow route contributions of the catchment model by combining information from measurements from the field site, discharge

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measurements of a small sub-catchment, and discharge measurements at the catchment outlet in a nested-scales model setup. This nested-scales model consist of thee sub-LGSI-models representing each of the scales: field-site, sub-catchment, and catchment. These model are connected by assuming that the parameters that describe the discharge response to groundwater depth are scale invariant (process-specific parameters, see Table 1), while the parameters that describe the spatial distribution of groundwater depths are assumed scale-specific (Table 1). The underlying hypothesis is that the differences between the observed hydrographs at the three scales are primarily an effect of a different spatial distribution of groundwater depths and resulting different active drainage areas.

All seven steps shown in Fig. 2 were followed to derive an ensemble of Behavioral Parameter Sets for the nested-scale model setup (BPS-N). First, a behavioral parameter set for the field site was created (first five steps of Fig. 2). Subsequently, we randomly generated new scale-specific parameter values for the sub-catchment until the model results for discharge and groundwater depth were satisfactory (criteria in Table 3). We also estimated a new constant drainage depth and drainage resistance, because the drainage depth and the time variant drainage resistance of the field site were specifically estimated for the three drains of the field site. Three drains probably do not represent the drain populations at larger scales. For the sub-catchment and catchment scale, we assumed that the many different pressure flushing (cleaning) dates of the tube drains and different drainage spacings led to a constant spatially averaged drainage resistance. Next, we re-estimated the scale-specific parameters for the entire catchment, and assumed the drainage depth and drainage resistance of the sub-catchment representative for the entire catchment. These seven steps were continued until 500 behavioral parameter sets were found (BPS-N). The flow route contributions to discharge during the entire field-site monitoring period and the parameter distributions for BPS-C and BPS-N were compared to assess the added value of introducing nested-scale measurements.

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2.6 Model validation

The BPS-C and the BPS-N were both validated for their ability to predict the catchment-scale discharge. For the validation we chose the period 1994–1995 for its high quality discharge data without data gaps and obvious measurement errors, and 1996–2001 for its episodes of extremely high discharges that are outside the discharge range of the calibration period.

A second model verification was performed by comparing nitrate loads calculated by BPS-C and BPS-N with measured nitrate loads. For this comparison, constant flow route concentrations were adapted from Van der Velde et al. (2010a) for tube drain flow (72 mg L⁻¹), overland flow (9 mg L⁻¹) and direct rainfall (9 mg L⁻¹). The groundwater flow concentration was estimated to be 50 mg L⁻¹, which corresponds to results of Rozemeijer et al. (2010c). Uncertainty in these concentrations are significant but are not accounted for in this comparison. Hence, we do not claim a real validation, but want to evaluate if the model is able to predict nitrate concentration behavior and to assess uncertainty propagation of flow route discharge uncertainty to nitrate load estimates.

3 Results and discussion

3.1 Nested-scale measurements

Figure 3 shows the results of the nested-scale discharge measurements. At the field site, tube drain discharge was by far the most important flow route. Over the entire period this flow routed contributed 78% of the total discharge. The remaining 22% is a mixture of overland flow during rainfall events (the sharp peaks in reservoir discharge of Fig. 3) and groundwater flow. The discharges of the sub-catchment and the entire catchment reflect the characteristic behavior of both the peaks measured by the in-stream reservoirs (overland flow) and the long recession tails of the tube drain discharge at the field scale.

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3.2 Field-site model

Van der Velde et al. (2009) reported a decrease in the simulated groundwater depth variance as the groundwater depth increased in their catchment-scale groundwater model. For the field site this finding is corroborated by observations for a wet and a dry day (Fig. 4). Approximating these distributions by normal distributions introduced only small errors (Fig. 4). Figure 5a shows the measured groundwater depths means and standard deviations for the 57 weekly groundwater depth surveys. The grey band in Fig. 5a represents the results of all behavioral parameter sets (BPS-FS) for the GDD-curve. This grey band is particularly narrow between average groundwater depths of 0.5 and 0.8 m (some of the data points are even outside it), indicating that the model results for storage and discharge are very sensitive to the GDD-curve in this range of average groundwater depths. GDD-curves outside the grey band, although they closely fit the observed GDD-data, did not yield behavioral models for some of the other criteria such as storage or discharge. In Fig. 5b we plotted the measured ponding volumes and the ponding curves of all BPS-FS. Because the measured ponding volumes are relatively uncertain (they are difficult to measure and we have only a few measurements) we allowed for a larger curve error (CE , Table 3). This resulted in the grey band in Fig. 5b.

Figure 6a shows the measured and modeled spatially averaged groundwater depth. The model results are accurate, but some of the moderate groundwater level peaks are underestimated. This also caused an underestimation of the tube drain discharge (Fig. 6b) during these moderate groundwater level peaks. Overall, Fig. 6 shows that the LGSI-model is able to accurately describe the average groundwater depth, tube drain flow, and reservoir discharge (Eq. 2) simultaneously. All three time series were simulated with a Nash-Sutcliffe (NS) coefficient (Nash and Sutcliffe, 1970) exceeding 0.8.

A comparison of the LGSI-model results with the results of Rozemeijer et al. (2010b), who used the same dataset and a fully distributed HydroGeosphere (Therrien et al., 2009) model to simulate flow routes during a single discharge event, demonstrate that

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the relatively simple LGSI-model concepts can simulate the discharges of individual flow routes equally well as the sophisticated HydroGeosphere model and hence constitute a very powerful tool for simulation and prediction of flow routes at a field site. Like Rozemeijer et al. (2010b), we found that measurements of both the storage of groundwater within the field and the corresponding discharge of flow routes are indispensable for an accurate model representation of the groundwater-surface water interaction.

3.3 Nested-scales model and model uncertainty

The discharges at all three nested-scales could be accurately described by parameter sets that share the same values for the process-specific parameters and differ only in scale-specific parameter values (Fig. 7). This result supports our hypothesis that scale effects in lowland hydrology can be attributed to scale differences in the shape of the groundwater table. These scale differences were quantified by the GDD-curves of the individual scales. Figure 8 shows the inferred ensemble of GDD-curves for the three nested scales. The differences between the field-site GDD-curve and the GDD-curve of the two catchment scales are much larger than those between the GDD-curves of both catchment scales. This is consistent with the small differences in the shape of the hydrographs between both catchment scales (Fig. 3).

The individual flow route contributions (the median contribution of BPS-N) to discharge are shown in Fig. 9. The relative overland flow and groundwater flow contributions to discharge increase with increasing scale, at the expense of tube drain discharge. Table 4 gives the 10–90 percentile estimates of flow route contributions for the entire simulation period (this period equals the field-site measurement period). The uncertainty in the flow route contributions at the field site is constrained by many different types of measurements (see also Fig. 6), but is much larger for the large scales, where less measurements were available. In Table 4 we also compared the uncertainty of the flow route contributions calculated by BPS-N and BPS-C. The uncertainty in groundwater flow, overland flow, and direct rainfall is significantly reduced by introducing nested scale measurements. In contrast, the uncertainty of the tube drain discharge could

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hardly be reduced because the field-site tube drain depth and tube drain resistance could not be transferred to larger scales. We re-estimated the tube drain-specific parameters for the sub-catchment and catchment-scale by assuming them to be equal for both scales, but even this assumption did not reduce the uncertainty.

3.4 Parameter distributions

Figure 10 shows the distribution of the behavioral parameter sets of all process-specific parameters. Since the prior distributions were uniform, sensitive parameters are identified by markedly non-uniform distributions. For the field site model (BPS-FS) the most sensitive parameters are α , D_{dr} , a_{dr} , L_f , and r_{ditch} . The sensitivity of a_{dr} signals that the tube drain resistance increases after tube drain cleaning. However, the insensitivity of b_{dr} and c_{dr} might indicate that the reduction in tube drain resistance during dry periods is of minor importance. The lateral inflow of groundwater, L_f , which is the closing term for the water balance, could be determined accurately around 0.6 mm day^{-1} . Surprisingly insensitive parameters are θ_s and u_{ET} . The insensitivity of u_{ET} signals that evapotranspiration reduction at our relatively wet (high groundwater tables) field site might not be very important. As long as the value of u_{ET} is less than two standard deviations (20 cm) below the lowest average groundwater water table, the modeled evapotranspiration reduction is small and u_{ET} does not affect the model results.

At the catchment scale (BPS-C) on the other hand, u_{ET} is the most sensitive parameter. At this scale this parameters closes the overall mass balance by increasing or reducing evapotranspiration (at the catchment scale there is not net lateral groundwater flow). Also m and r_{ex} are relatively sensitive as they directly control the discharge, which is the only calibration objective. All other parameters are insensitive and the uncertainty in flow route contribution is largely determined by the boundaries of the prior distributions.

For the nested-scales model (BPS-N) we sought process-specific parameter sets that can describe all three scales simultaneously. Figure 10 shows that the parameter distributions of BPS-N combine the constraints of the distribution of both BPS-FS and

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BPS-C. The added value of including nested-scale measurements to reduce parameter uncertainty is apparent for almost all process-specific parameters.

Figure 11 shows the distributions of the scale-specific parameters and again the reduction in parameter uncertainty by introducing nested-scale measurements is clear.

Note that the distribution of σ_{\min} tends to high values exceeding the preset boundaries in Table 2 that were determined from a detailed DEM. Under dry conditions, the groundwater level is almost parallel to the soil surface at the resolution of the DEM (5 m). Variations in the groundwater depth under such conditions emanate largely from local variations in the soil surface elevation that are too small to appear in the phreatic level. However, under dry conditions a few very deep incisions of the stream produce most discharge. Around these incisions, the groundwater depth necessarily decreases sharply to zero at the stream bank, and these deviating groundwater depths produce outliers from the normal distribution valid for the rest of the catchment. As a consequence, the calibration tried to increase the groundwater depth variation (and thereby the range of σ_{\min}) under dry conditions to be able to generate low discharges. Because these discharges are low, the effect of underestimating discharges during dry conditions on the entire water balance of the catchment is small.

In general, both Figs. 10 and 11 suggest that that the LGSI-model is highly overparameterized when the model is only calibrated on discharge, because almost all parameters of BPS-C are insensitive (uniform distributions). However, nested-scale measurements and the assumption that scale differences are driven only by the groundwater table increases the parameter sensitivity and allows most parameters to be conditioned.

3.5 Model validation

The BPS-N performed slightly better than BPS-C for both validation periods. For the period 1994–1995 the BPS-N yielded an average *NS*-coefficient of 0.90, against 0.85 for the BPS-C. For the validation period 1996–2001 the average *NS*-coefficients were 0.79 for BPS-N and 0.73 for BPS-C. Although these may seem minor improvements in model performance when weighted against the efforts involved in the

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nested-scale monitoring, these model improvements are especially apparent in extreme discharges beyond the range of the calibration dataset. Figure 12 shows the validation results of the four most extreme discharge events during the period 1996–2001. From all events it is clear that the BPS-N much better predicted discharge than BPS-C (particularly the magnitude of the peaks), with far smaller uncertainty ranges. During the discharge events in Fig. 12c, which are the highest discharges measured in the past 20 years, the measured maximum discharge was more than twice the maximum discharge of the calibration period. During this period some of the BPS-C overestimated the discharge by a factor 3, while the BPS-N all predicted discharges close to the measured discharge.

The model improvement achieved by conditioning the model on nested-scale measurements is also apparent from the comparison between simulated and measured nitrate concentrations and nitrate loads (Fig. 13). Assuming constant flow route concentrations yielded good descriptions of the nitrate concentration fluctuations at the catchment outlet for both models (BPS-C and BPS-N). But conditioning on nested-scale data reduced the uncertainty in cumulative load estimates by 50%. This shows how vital accurate estimations of flow route discharges are for estimating solute loads towards downstream surface water bodies.

We argue that, because the nested scale measurements combined with the nested-scale model could partly constrain the uncertainty in flow route discharges (Table 4), the BPS-N have a better chance of describing ‘the right discharge for the right reason’ (Kirchner, 2006), i.e., the correct combination of flow routes. This was demonstrated by the better peak discharge predictions during the validation period and reduced uncertainty in nitrate load estimates of the nested-scales model (BPS-N).

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4 Conclusions

Detailed and unique flux measurements at a pasture field site allowed us to formulate and calibrate our parsimonious LGSI-model. Even the very non-linear process of saturated overland flow was adequately simulated by the field-site model. An exceptional feature of this model is that the model concepts were designed around the available measurements (Van der Velde et al., 2009). Consequently, the parameters that describe the discharge and storage processes could all be conditioned on measurements. This yielded a field-site model that accurately described both storage and fluxes simultaneously.

The combined nested-scale measurement and model setup made it possible to combine discharge information of the field scale, a small sub-catchment, and the entire catchment. We demonstrated that the differences between hydrographs at the three scales could all be described by only changing the Groundwater Depth Distribution (GDD) curve, even though the hydrographs were markedly different. This result supports our hypothesis that scale effects on discharge in lowland catchments are primarily an effect of differences in the spatial distributions of groundwater depths between different scales. Still, the range of GDD-curves that yielded good model results for the catchment scales was wide. This emphasizes the importance of spatially distributed groundwater depth monitoring to further condition these GDD-curves. This should lead to an even more solid foundation supporting the physical representation of the catchment's hydrology, and hence to more reliable results.

Tube drain effluent is the most important route for nitrate towards the surface water network in lowland catchments. We were able to measure tube drain discharge at the field site and we concluded that almost 80% of the water (Van der Velde et al., 2010a) and 92% of the nitrate (Rozemeijer et al., 2010c) was transported by tube drains. It is by no means trivial to extrapolate these field-scale findings to the entire catchment. Our combined nested-scales observation and modeling approach could narrow down the contribution of tube drain discharge to the discharge of a sub-catchment of 0.4 km²

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to 34–61% of the total discharge. For the entire catchment of 6.5 km² 25–50% of the discharge originated from tube drains. These results not only demonstrate that we need to be careful extrapolating field experiment results to entire catchments but also show that nested-scale measurements are essential to understand and quantify the flow route contributions to the discharge of a catchment.

In this paper we demonstrated the potential of combined nested-scale monitoring and modeling for the Hupsel Brook catchment. However, many of our findings can be generalized. First of all, we showed that detailed field-site measurements of storage and flow routes provide the process-understanding that is needed to develop a model structure that adequately describes the catchment-specific flow routes. Secondly, we demonstrated that the combination of a relatively short period of nested-scale measurements with nested-scale models significantly constrains uncertainty in the contributions of groundwater flow, overland flow, and direct rainfall into surface waters, which in turn significantly reduces uncertainty in nitrate load estimates. Finally, we showed that conditioning parameter sets on nested-scale measurements considerably improves discharge predictions compared to parameter sets constrained on discharge only. Model calibration on nested-scale measurements may not yield models with better calibration-statistics than models that are calibrated on catchment discharge alone, but the nested-scales model approach yields models that are able to predict (peak) discharges during validation periods more accurately. Improved quantifications and predictions of nitrate loads and peak discharges make the efforts involved in nested-scale monitoring worthwhile.

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Appendix A

Notation

A1 Abbreviations

| | |
|-----------------------|--|
| LGSI-model | Lowland Groundwater-Surface water Interaction model developed by Van der Velde et al. (2009) |
| GDD-curve | Groundwater Depth Distribution curve. Curve that relates the spatial standard deviation of the groundwater depth to its spatial average. |
| Ponding-curve | The relation between spatially averaged groundwater depth and the volume of ponds and surface waters. |
| BPS | Ensemble of 500 Behavioral Parameter Sets. |
| BPS-FS, BPS-C, BPS-N: | BPS for each of the three models: field-site, catchment and nested-scales model respectively. |

A2 Symbols

| | |
|-----------------------|--|
| $A_{dr} [L^2]$ | Area within the catchment that is drained by subsurface tubes |
| $A_s [L^2]$ | Area within the catchment covered with surface water |
| $A_{tot} [L^2]$ | Catchment area |
| $a_{dr} [-]$ | Rate with which r_{dr} increases during wet periods |
| $b_{dr} [T^{-1}]$ | Fractional rate with which r_{dr} decreases during dry periods |
| $c_{dr} [L^3 T^{-1}]$ | Threshold tube drain discharge: below this discharge r_{dr} decreases, above this discharge r_{dr} increases |
| $CDE [-]$ | Cumulative discharge error, difference between cumulative measured and modeled discharge |

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| CE [-] | Curve error, difference between measured data and the modeled GDD-curve or ponding-curve |
| D_{dr} [L] | Tube drain depth |
| e_{pot} [$L T^{-1}$] | Potential evapotranspiration |
| ET_{act} [$L T^{-1}$] | Actual evapotranspiration |
| fu [L^{-1}] | Normal distribution function of groundwater depths |
| Fu [-] | Cumulative distribution function of groundwater depths |
| Fu^{-1} [-] | Inverse cumulative distribution function of groundwater depths |
| GE [L] | Average groundwater depth error between measured and modeled groundwater time series. |
| h [L] | Height above the groundwater table |
| L_f [$L T^{-1}$] | The constant lateral inflow of groundwater at the field site |
| m [-] | Fraction of groundwater levels above the soil surface that remain on the soil surface to constitute surface storage. |
| NS [-] | Nash-Sutcliff (Nash and Sutcliff, 1970) coefficient for time series. |
| P [$L T^{-1}$] | Rainfall |
| P_Q [$L T^{-1}$] | Rainfall on ponded surface or surface waters |
| Q [$L T^{-1}$] | Discharge at catchment outlet |
| Q_{grw} [$L T^{-1}$] | Groundwater flow for sub-catchment and entire catchment |
| $Q_{grw,field}$ [$L T^{-1}$] | Groundwater flow towards ditch at field site |
| Q_{ov} [$L T^{-1}$] | Overland flow |
| Q_{res} [$L T^{-1}$] | Discharge as measured by the in-stream reservoirs |
| r_{ditch} [T] | Resistance of the field site to groundwater flow towards the ditch. |
| r_{dr} [T] | Tube drain resistance |
| r_{ex} [T] | Groundwater exfiltration resistance |
| S_{sat} [L] | Storage in saturated zone normalized by area |
| S_{surf} [L] | Storage in ponds and surface water normalized by area |

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| | |
|----------------------------|---|
| S_{unsat} [L] | Storage in unsaturated zone normalized by area |
| u [L] | Groundwater depth |
| $\langle u \rangle$ [L] | Spatial average of the groundwater depth |
| u_{ditch} [L] | Depth of the field-site ditch relative to the mean surface elevation of the field site |
| u_{ET} [L] | Groundwater depth at which the actual evapotranspiration drops from e_{pot} to reduction depth |
| $u_{\text{s max}}$ [L] | Average groundwater depth at which the standard deviation of the groundwater depths is at its maximum |
| α [L], n [-] | Van Genuchten (1980) parameters that describe the soil water retention curve |
| σ_{diff} [L] | Maximum increase in the standard deviation of the groundwater depth |
| σ_{min} [L] | Minimal groundwater depth standard deviation |
| σ_u [L] | Groundwater depth standard deviation corresponding to a certain $\langle u \rangle$ |
| θ_s [-] | Average porosity between highest and lowest groundwater table [-] |

Appendix B

LGSI-model expressions

The overall water balance of the model normalized by area and zero lateral influx is given by:

$$\frac{\partial S_{\text{sat}}(t)}{\partial t} + \frac{\partial S_{\text{unsat}}(t)}{\partial t} + \frac{\partial S_{\text{surf}}(t)}{\partial t} = P(t) - \text{ET}_{\text{act}}(t) - Q(t) \quad (\text{B1})$$

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with saturated zone storage, $S_{\text{sat}} [L]$, unsaturated zone storage, $S_{\text{unsat}} [L]$, surface storage in streams, ditches and ponds, $S_{\text{surf}} [L]$, the rainfall flux, $P [L T^{-1}]$, actual evapotranspiration, $ET_{\text{act}} [L T^{-1}]$, and discharge, $Q [L T^{-1}]$. The storage terms on the left-hand side of Eq. (A1) are described as a function of the distribution of groundwater depths, $f_u [L^{-1}]$. The change in saturated storage is expressed by the inverse of the change in unsaturated zone volume:

$$\frac{\partial S_{\text{sat}}(t)}{\partial t} = -\theta_s \frac{\partial}{\partial t} \left(\int_0^{\infty} f_u(t) u du \right) \quad (\text{B2})$$

with the groundwater depth, $u [L]$, the spatial averaged soil porosity, $\theta_s [-]$, the distribution in groundwater depths, $f_u [L^{-1}]$, and the total unsaturated zone volume normalized by the catchment area $\int_0^{\infty} f_u(t) u du$. Note that the positive integration bounds implicate that the unsaturated zone does not exist for negative groundwater depths (ponding).

The volume of water stored in the unsaturated zone is described with a Van Genuchten (1980) relationship for soil moisture in an unsaturated zone at hydrostatic equilibrium. The change in unsaturated zone storage is described by:

$$\frac{\partial S_{\text{unsat}}(t)}{\partial t} = \theta_s \frac{\partial}{\partial t} \left(\int_0^{\infty} f_u(t) \int_0^u [1 + (\alpha h)^n]^{\frac{1}{n}} - 1 dh du \right) \quad (\text{B3})$$

The height above the groundwater level is denoted by $h [L]$, and $\alpha [L^{-1}]$ and $n [-]$ are the Van Genuchten parameters, with the residual volumetric water content equal to zero.

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Water stored on the soil surface in ditches and ponds is described by a fixed fraction, m [-], of the total volume of groundwater heads above the soil surface:

$$S_{\text{surf}}(t) = -m \int_{-\infty}^0 f_u(t) u du \quad (\text{B4})$$

The change in surface storage is given by:

$$\frac{\partial S_{\text{surf}}(t)}{\partial t} = -m \frac{\partial}{\partial t} \left(\int_{-\infty}^0 f_u(t) u du \right) \quad (\text{B5})$$

Deep groundwater levels reduce the potential evapotranspiration. We chose a single cutoff level, u_{et} , below which no evapotranspiration is possible and above which potential evapotranspiration, e_{pot} , occurs. This leads to the following expression for evapotranspiration:

$$\text{ET}_{\text{act}}(t) = e_{\text{pot}}(t) \int_{-\infty}^{u_{\text{et}}} f_u(t) du \quad (\text{B6})$$

Furthermore, we assumed that a specific volume of groundwater is always stored in the same way (i.e., the moments of the distribution of groundwater depths only depend on the amount of storage and are not hysteretic). We are not interested in the exact configuration of storage within the catchment, and therefore assumed a normally distributed groundwater depth with an empirical relationship relating the standard deviation of groundwater depths, σ_u [L] to the spatial average of the groundwater depth $\langle u(t) \rangle$:

$$\sigma_u = \sigma_{\text{diff}} \cdot e^{-\left(\frac{\langle u(t) \rangle - u_{\text{sd max}}}{b}\right)^2} + \sigma_{\text{min}} \quad (\text{B7})$$

Van der Velde et al. (2009) showed that this relation holds for field- and catchment-scales.

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B1 Storage-discharge relationships

The contribution of specific flow routes to overall discharge largely determines the discharge quality. Therefore we subdivided the total discharge, Q , into four flow routes with distinctly different water chemistry:

$$Q(t) = Q_{\text{drain}}(t) + Q_{\text{grw}}(t) + Q_{\text{ov}}(t) + P_Q(t) - E_Q(t) \quad (\text{B8})$$

with Q_{drain} [$L T^{-1}$] groundwater discharge by tube drains, Q_{ov} [$L T^{-1}$], discharge by overland flow, and Q_{grw} [$L T^{-1}$], discharge of phreatic groundwater flow by ditch and stream drainage. Rain falling directly on the surface water network is denoted by P_Q [$L T^{-1}$] and evaporation from the surface water network is denoted by E_Q [$L T^{-1}$].

The tube drain discharge is calculated from the groundwater depth distribution by:

$$Q_{\text{drain}}(t) = \frac{A_{\text{dr}}}{r_{\text{dr}} A_{\text{tot}}} \int_{F_u^{-1}(A_s/A_{\text{tot}})}^{D_{\text{dr}}} f_u(t) \cdot (D_{\text{dr}} - u) du \quad (\text{B9})$$

with A_{dr} [L^2] the surface area occupied by tube drains, A_{tot} the catchment surface area, r_{dr} [T] the resistance of the soil to tube drain discharge and D_{dr} [T] the average depth of the tube drains. The fraction of catchment surface that is wet but has no tube drains, such as the surface area of ditches and streams, is denoted by A_s . This fraction is important under dry conditions when tube drainage stops and groundwater drainage by ditches and the stream takes over.

Van der Velde et al. (2009) made no distinction between overland flow and groundwater flow towards ditches and streams. They reasoned that the physical principles driving both fluxes are equal: groundwater level gradients driving water from the soil into surface waters or ponds. In this study we follow the same line of reasoning but we want to separate both fluxes, because the two fluxes have distinctly different effects on the water quality. We hypothesize that under wet conditions, first all ditches

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start draining and only when the catchment becomes so wet that the drainage area, $F_u(0) = \int_{-\infty}^0 f_u(t) du$, exceeds the surface area occupied by ditches, A_s , overland flow starts to occur. Now we can subdivide the groundwater flux into groundwater flow towards ditches and overland flow by the corresponding drainage area:

$$\begin{aligned}
 Q_{\text{grw}}(t) + Q_{\text{ov}}(t) &= \frac{m-1}{r_{\text{ex}}} \int_{-\infty}^0 f_u(t) \cdot u du \\
 Q_{\text{grw}} &= \frac{m-1}{r_{\text{ex}}} \int_{-\infty}^{\min\left(F_u^{-1}\left(\frac{A_s}{A}\right), 0\right)} f_u(t) \cdot u du \\
 Q_{\text{ov}} &= \frac{m-1}{r_{\text{ex}}} \int_{\min\left(F_u^{-1}\left(\frac{A_s}{A}\right), 0\right)}^0 f_u(t) \cdot u du
 \end{aligned} \tag{B10}$$

with $r_{\text{ex}} [T]$ the resistance of the soil to groundwater flow towards surface water and ponds. The term $\min\left(F_u^{-1}\left(\frac{A_s}{A}\right), 0\right)$ divides the negative part of the distribution of groundwater depth f_u (i.e. areas with ponding) in two areas: an area with groundwater flow and an area with overland flow, where $F_u^{-1}\left(\frac{A_s}{A}\right) < 0$.

The amount of rain that falls on the active drainage area and is discharged immediately is:

$$P_Q(t) = p(t) \int_{-\infty}^0 f_u(t) du \tag{B11}$$

The evaporation of surface water is:

$$E_Q(t) = e_{\text{pot}}(t) \int_{-\infty}^0 f_u(t) du \tag{B12}$$

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Model error expressions

Four error-terms divide the parameters space in behavioral and non-behavioral parameter sets. The Curve Error term quantifies the average normalized distance between the measurements and the modeled GDD-curve or Ponding curve:

$$CE = \frac{1}{n} \sum_{i=1}^n \min \left(\sqrt{\left(\frac{\langle u \rangle_i - \langle u \rangle_c}{\overline{\langle u \rangle}} \right)^2 + \left(\frac{y_i - y_c}{\bar{y}} \right)^2} \right), \text{ with } y_c = f(\langle u \rangle_c) \quad (C1)$$

The minimum function identifies the minimum normalized distance between the measurements and the model-curve. The number of measurements is denoted by n ; $\langle u \rangle_i$ is the spatially averaged groundwater depth at the time measurement i was obtained; $\langle u \rangle_c$ is a spatially averaged groundwater depth defined by the GDD-curve or the Ponding-curve; $\overline{\langle u \rangle}$ is the temporal average of the measured spatially averaged groundwater depth (i.e., the groundwater depth averaged over space and time); y_i is the measured variable (the standard deviation of the groundwater depth for the GDD-curve, and the ponding volume for the Ponding-curve); y_c is the same variable defined by the model curve, and \bar{y} the temporal average of the measured values of this variable.

The second error term quantifies the error in the total water balance:

$$CDE = \left| 1 - \frac{\sum_{i=1}^n Q_{\text{mod},i}}{\sum_{i=1}^n Q_{\text{meas},i}} \right| \quad (C2)$$

With $Q_{\text{mod},i}$ [$L^3 T^{-1}$], the modeled discharge corresponding to measured discharge $Q_{\text{meas},i}$ [$L^3 T^{-1}$]. The dynamics of groundwater depth and discharge time series

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(both defined by the variable V in the following equation) are evaluated by the Nash-Sutcliffe statistic (Nash and Sutcliffe, 1970)

$$NS = 1 - \frac{\sum_{i=1}^n (V_{\text{meas},i} - V_{\text{mod},i})^2}{\sum_{i=1}^n (V_{\text{meas},i} - \overline{V_{\text{meas}}})^2} \quad (\text{C3})$$

with $\overline{V_{\text{meas}}}$ [$L^3 T^{-1}$] the average measured discharge or groundwater depth.

The simulated groundwater dynamics for both catchment scales are compared with a single measured groundwater level time series. This comparison is evaluated by:

$$GE = \frac{1}{n} \sum_{i=1}^n fGE_i \quad (\text{C4})$$

with fGE [-] a measure of the degree to which a measured groundwater depth, $u_{\text{meas},i}$ [L], is outside the acceptable bounds ($UI_{\text{min},i}$ [L] and $UI_{\text{max},i}$ [L]) of the modeled groundwater depth distribution:

$$fGE_i = u_{\text{meas},i} - UI_{\text{max},i} \text{ if } u_{\text{meas},i} > UI_{\text{max},i}$$

$$fGE_i = UI_{\text{min},i} - u_{\text{meas},i} \text{ if } u_{\text{meas},i} < UI_{\text{min},i}$$

$$fGE_i = 0 \text{ if } UI_{\text{min},i} < u_{\text{meas},i} < UI_{\text{max},i}$$

The acceptable bounds, UI_{min} and UI_{max} , are a fixed quantile of the modeled distribution and are recalculated for each time step, i , based on an estimate of the representativity of a location where groundwater depths are measured for a certain area. We estimated that the measured average groundwater depth at the field site should always be within the 0.20–0.80 percentile of all groundwater depths in the sub-catchment and within 0.1–0.90 of the groundwater depths of the entire catchment.

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Table 1. LGSi-Model basics and parameters. The process formulations are point-scale model equations. The catchment-scale equations are obtained by integration over the groundwater depth distribution within appropriate integration bounds (see Appendix B).

| Process | Formulation | Process-specific parameters |
|---|---|---|
| Unsaturated zone storage (s_{unsat}) | $s_{\text{unsat}} = \theta_s \int_0^u [1 + (\alpha h)^n]^{\frac{1}{n}-1} dh \text{ for } u > 0$ $s_{\text{unsat}} = 0 \text{ for } u < 0$ | u : Groundwater depth [L] θ_s : Porosity [-] α, n : Van Genuchten parameters [L], [-] h : Height above water table [L] |
| Saturated zone storage (s_{surf}) | $s_{\text{surf}} = -m \cdot u \text{ for } u < 0$ $s_{\text{surf}} = 0 \text{ for } u > 0$ | m : Fraction of ponding [-] |
| Evapo-transpiration (e_{act}) | $e_{\text{act}} = e_{\text{pot}} \text{ for } u < u_{\text{ET}}$ $e_{\text{act}} = 0 \text{ for } u > u_{\text{ET}}$ | e_{pot} : Potential evapotranspiration [$L \cdot T^{-1}$] u_{ET} : Evapotranspiration reduction depth [L] |
| Overland (q_{ov}), Groundwater flow (q_{grw}) | $q_{\text{grw,ov}} = \frac{(m-1) \cdot u}{r_{\text{ex}}} \text{ for } u < 0$ $q_{\text{grw,ov}} = 0 \text{ for } u > 0$ | r_{ex} : Exfiltration resistance [T] |
| Tube drain flow (q_{dr}) | $q_{\text{dr}} = \frac{D_{\text{dr}} - u}{r_{\text{dr}}} \text{ for } u < D_{\text{dr}}$ $q_{\text{dr}} = 0 \text{ for } u > D_{\text{dr}}$ | D_{dr} : Tube drain depth [L] r_{dr} : Tube drain resistance [T] |
| Scale | Formulation | Scale-specific parameters |
| GDD-curve | $\sigma_u = \sigma_{\text{diff}} \cdot e^{-\left(\frac{u - u_s \text{ max}}{b}\right)^2} + \sigma_{\text{min}}$ | σ_u : Spatial groundwater depth st. dev. [L] $\langle u \rangle$: Spatial average grw. depth [L] σ_{min} : Minimal grw. depth st. dev. [L] σ_{diff} : Maximum increase in grw. depth st. dev. [L] $u_s \text{ max}$: Average grw. depth with maximum grw. depth st. dev. [L] |
| Surfaces | – | A_{tot} : Catchment area [L^2] A_{dr} : Area with tube drainage [-] A_s : Area with surface water [-] |

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Table 2. Estimated Process-specific and Scale-specific parameter ranges.

| Process-specific parameters | | Scale-specific parameters | | | |
|-----------------------------|---|---|----------------------------|--|--|
| | | Field site | Sub-catchment | Catchment | |
| α | 1–2 m ⁽¹⁾ | σ_{\min} | 0.06–0.13 m ⁽²⁾ | 0.14–0.22 m ⁽²⁾ | 0.2–0.30 m ⁽²⁾ |
| n | 1–6 ¹ | σ_{diff} | 0.1–0.6 m ⁽³⁾ | 0.1–0.6 m ⁽³⁾ | 0.1–0.6 m ⁽³⁾ |
| θ_s | 0.35–0.45 ⁽¹⁾ | $u_{s \text{ max}}$ | 0.1–0.6 m ⁽³⁾ | 0.1–0.6 m ⁽³⁾ | 0.1–0.6 m ⁽³⁾ |
| M | 0.05–0.7 ⁽³⁾ | B | 0.1–0.6 m ⁽³⁾ | 0.1–0.6 m ⁽³⁾ | 0.1–0.6 m ⁽³⁾ |
| u_{ET} | 1–2 m ⁽³⁾ | $A_{\text{dr}}/A_{\text{tot}}$ | 1.0 | 0.7–0.9 ⁽⁴⁾ | 0.4–0.6 ⁽⁴⁾ |
| r_{ex} | 0.1–10 d ⁽³⁾ | A_s/A_{tot} | 0 | 0.0054–0.0066 ⁽⁴⁾ | 0.009–0.011 ⁽⁴⁾ |
| r_{ditch} | 500–4000 d ⁽³⁾ | A_{tot} | 7700–9000 m ² | 0.36–0.48 Km ² ⁽⁴⁾ | 6.0–7.3 Km ² ⁽⁴⁾ |
| u_{ditch} | 1.05 m ⁽⁵⁾ | ⁽¹⁾ Soil parameter estimates from Wösten et al. (2001) | | | |
| D_{dr} | 0.75–0.95 m ⁽⁵⁾ | ⁽²⁾ DEM | | | |
| r_{dr} | 100–300 d ⁽³⁾ | ⁽³⁾ Rough estimates | | | |
| a_{dr} | 0–2.2 ⁽³⁾ | ⁽⁴⁾ Topographic maps and field survey | | | |
| b_{dr} | 0–0.14 d ⁻¹ ⁽³⁾ | ⁽⁵⁾ Field-site measurements | | | |
| c_{dr} | 0–0.8 mm day ⁻¹ ⁽³⁾ | | | | |
| L_f | 0–0.8 mm day ⁻¹ ⁽³⁾ | | | | |
| Mp | 0.95–1.05 ⁽³⁾ | | | | |
| Me | 0.95–1.05 ⁽³⁾ | | | | |

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Table 3. The cutoff criteria for behavioral model runs. Model runs are assigned behavioral when they meet to all “goodness of fit” criteria. Expressions for the error terms are given in Appendix B.

| | Field site (storage) | | | Field site (fluxes) | | | Catchment |
|---|----------------------|---------------|------------|---------------------|-----------|------------------------|------------------------|
| | GDD-curve | Ponding curve | Grw. depth | Tube drain | Reservoir | Sub-catchment | |
| Curve Error: <i>CE</i> | 0.07 | 0.2 | – | – | – | – | – |
| Cumulative discharge error: <i>CDE</i> | – | – | – | < 5% | < 10% | < 8% | < 8% |
| Nash-Sutcliff coeff. for time series: <i>NS</i> | – | – | > 0.9 | > 0.8 | > 0.8 | > 0.85 | > 0.75 |
| Average Groundwater depth error: <i>GE</i> | – | – | – | – | – | < 1 cm (0.2–0.8 p)* | < 1 cm (0.1–0.9 p)* |

* The lower and upper quantile of the modeled groundwater depth distribution that is assumed to envelope the measured groundwater depth at the field site. The *GE* gives the maximum average difference between the measured groundwater depth and the modeled envelope.

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Table 4. Calculated flow route contribution (0.1–0.9 quantiles) of BPS-N and BPS-C. The contribution is calculated over the period November 2008 through December 2009.

| | BPS-N | | | BPS-C |
|------------------|------------|---------------|-----------|-----------|
| | Field-site | Sub-catchment | Catchment | Catchment |
| Tube drain flow | 0.76–0.79 | 0.34–0.61 | 0.25–0.50 | 0.21–0.51 |
| Groundwater flow | 0.10–0.15 | 0.06–0.16 | 0.12–0.27 | 0.14–0.50 |
| Overland flow | 0.04–0.07 | 0.24–0.42 | 0.27–0.41 | 0.18–0.37 |
| Direct rainfall | 0.03–0.05 | 0.07–0.11 | 0.08–0.11 | 0.03–0.10 |

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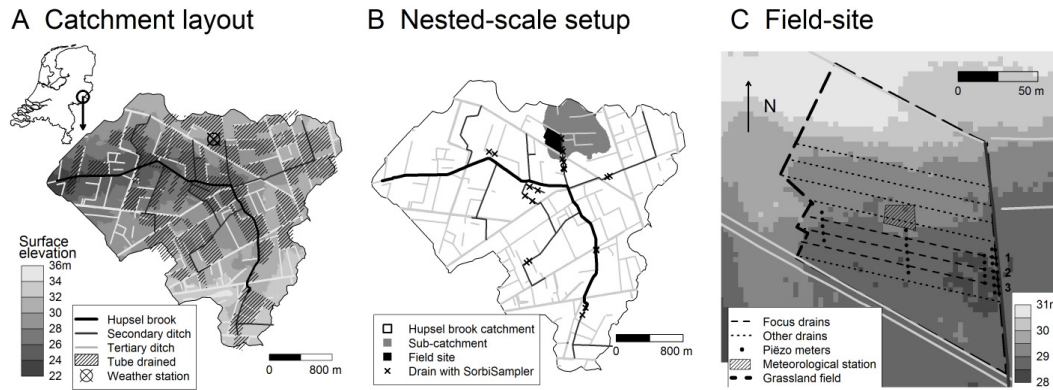


Fig. 1. Hupsel Brook catchment and nested-scale measurement setup.

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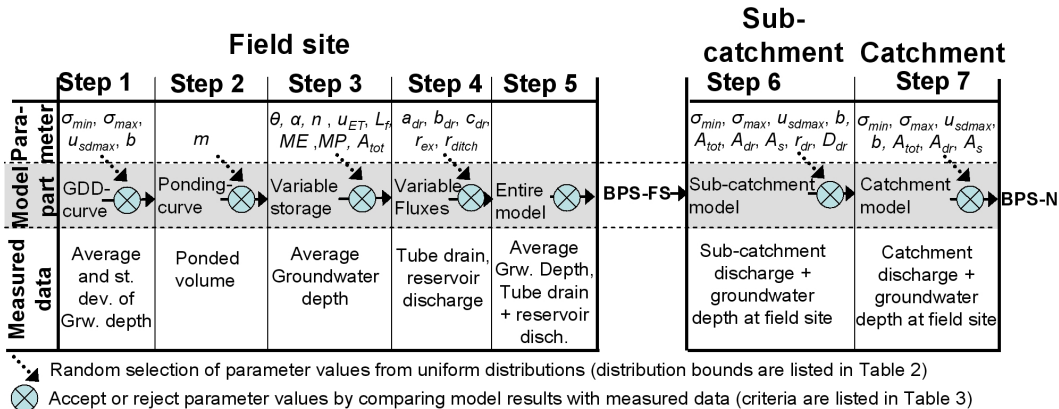


Fig. 2. Procedure for derivation of behavioral parameter sets for fields-site and nested-scales model. The first five steps yield behavioral parameter set for the field site (BPS-FS). All seven steps yield behavioral parameter sets for the nested scale model setup (BPS-N). The parameters are explained in Table 1.

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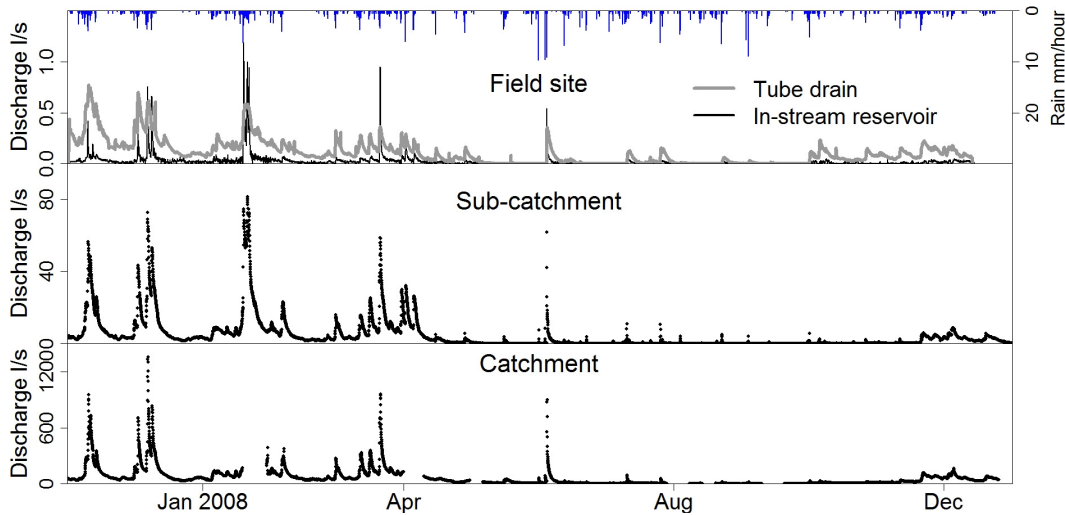


Fig. 3. Measured nested-scale discharges in response to rainfall measured at the field site.

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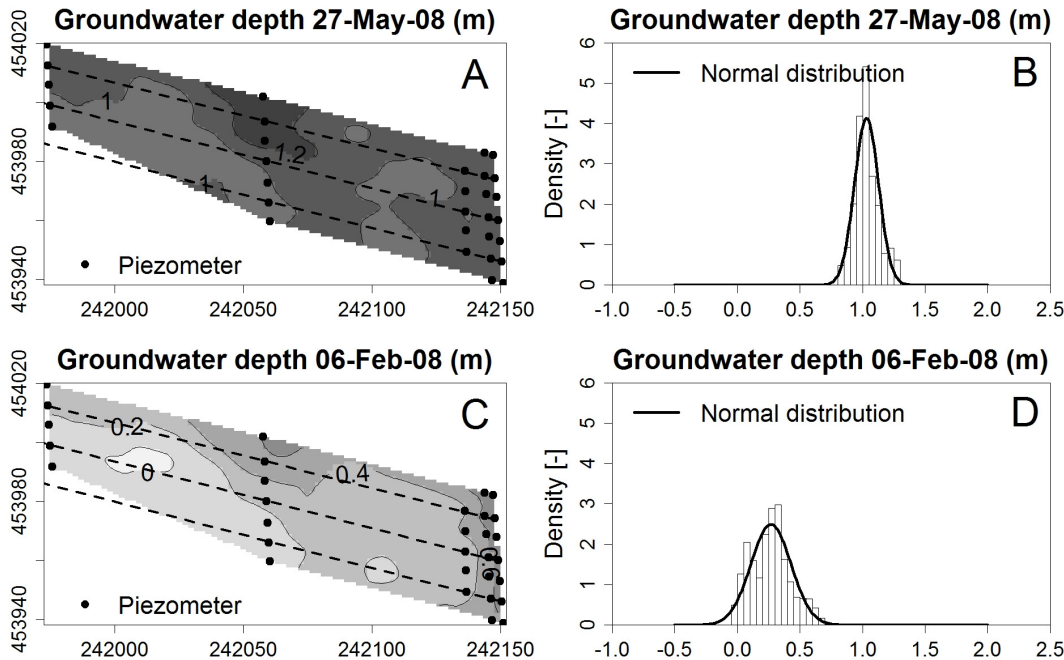


Fig. 4. Map of field-site groundwater depth for a dry (A) and a wet (C) day and the corresponding groundwater depth distributions – (B) and (D).

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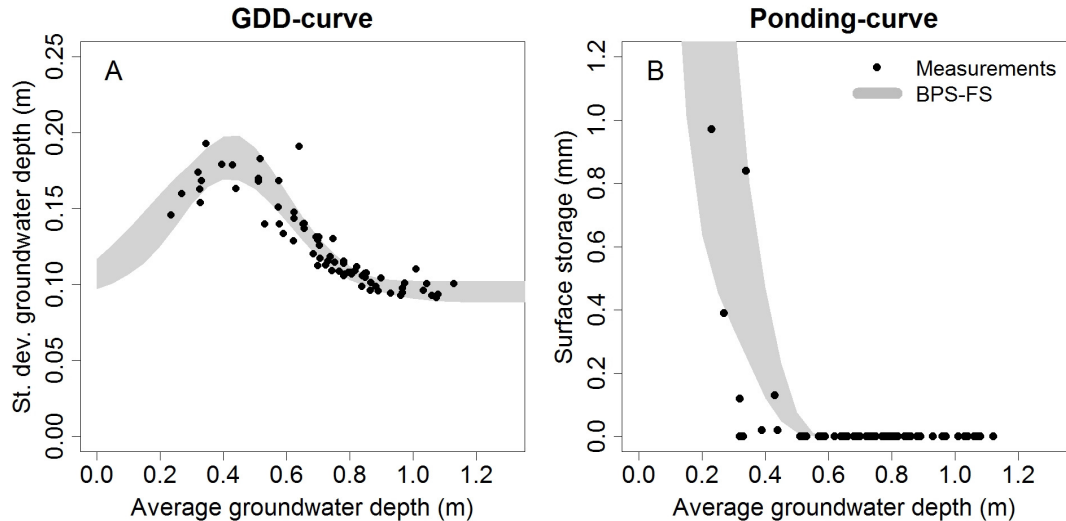


Fig. 5. Measured and simulated groundwater depth distribution curve (GDD-curve) **(A)** and Ponding curve **(B)** of the field-site. The grey area represents the ensemble of behavioral parameter sets of the field-site model (BPS-FS).

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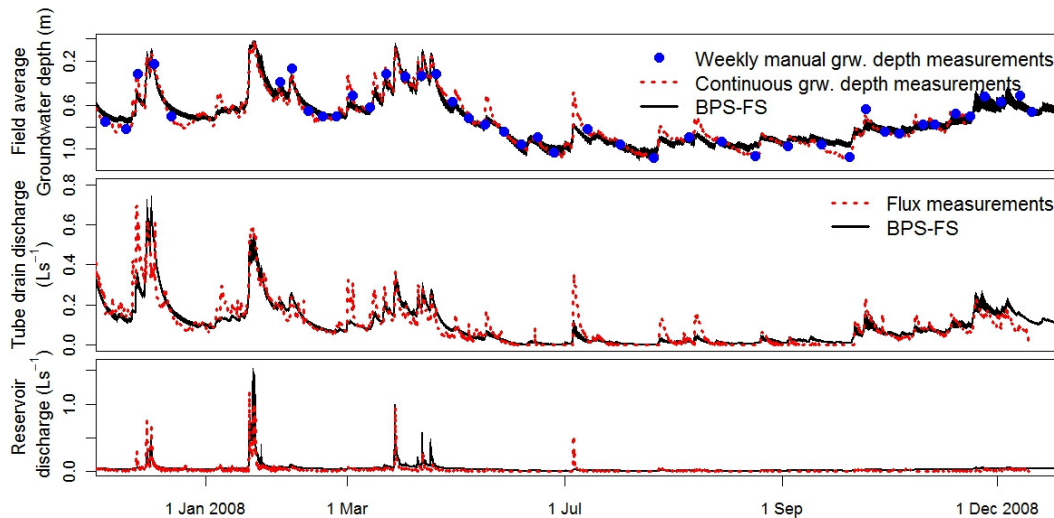


Fig. 6. Measurements and simulation results of the field site model (BPS-FS) for the spatially averaged groundwater depth (**A**), tube drain discharge (**B**), and reservoir discharge – combined flux of overland flow and groundwater flow, (**C**) – of the field-site. The black band gives the results of all behavioral parameter sets (BPS-FS).

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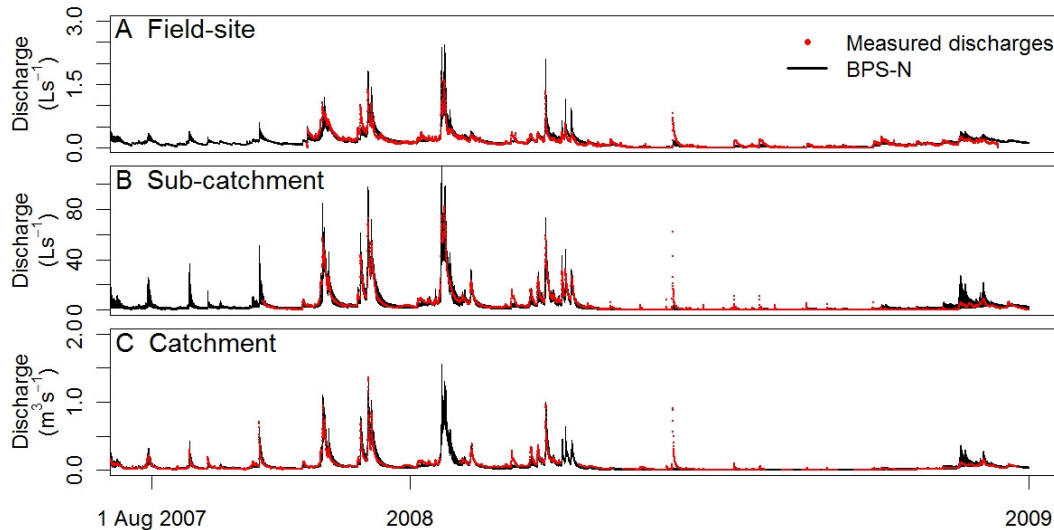


Fig. 7. Measurements and simulation results the nested-scales model for total discharges of the field-site **(A)**, sub-catchment **(B)** and entire catchment **(C)**. The black band gives the results of all behavioral parameter sets (BPS-N).

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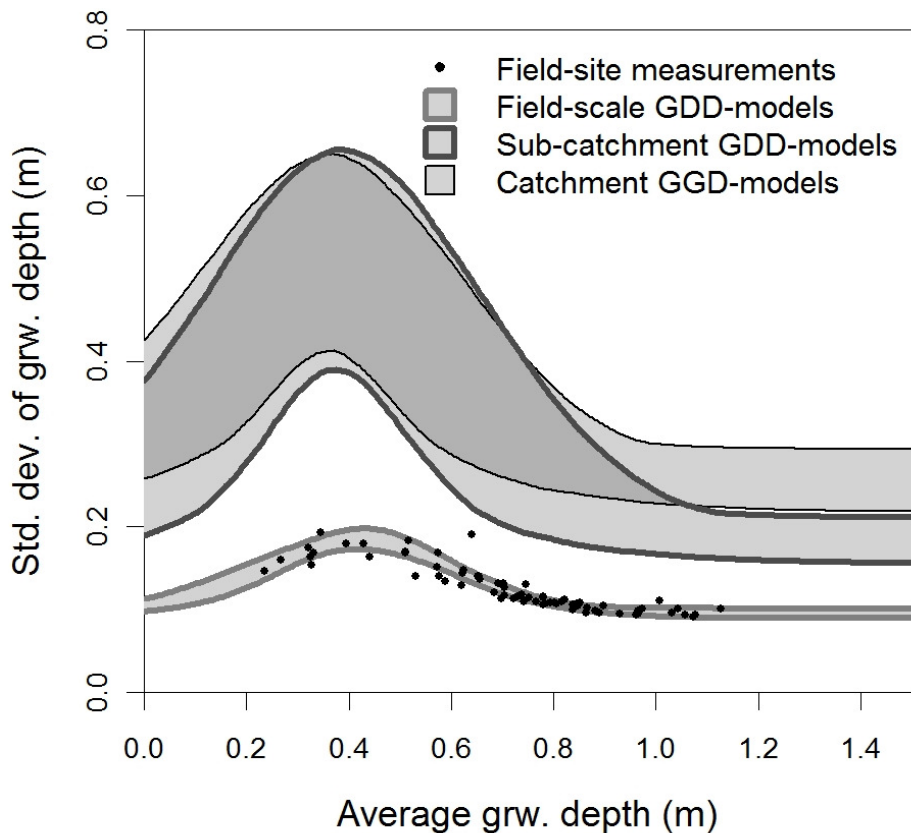


Fig. 8. Bandwidth of behavioral GDD-curves for the three scales of the nested-scales model (BPS-N). The dark grey area indicates overlap between ensembles of GDD-curves.

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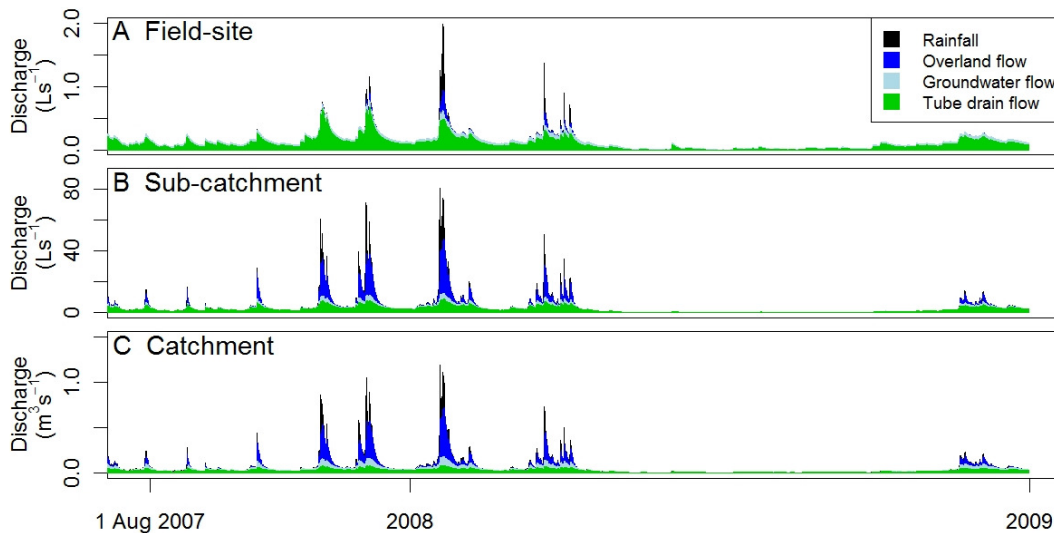


Fig. 9. Contributions of flow routes to total discharge. The displayed contribution is the median of contribution of all behavioral parameter sets (BPS-N).

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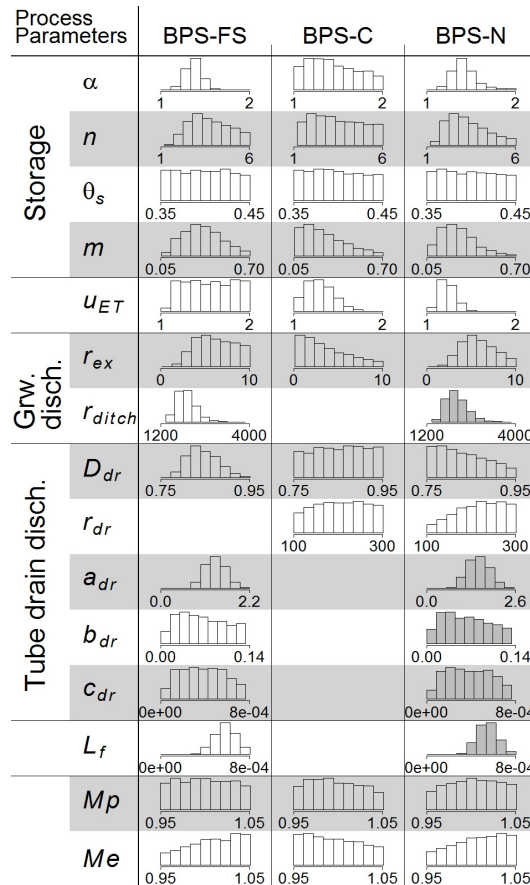


Fig. 10. Process-specific parameter distributions for the three behavioral parameter sets: BPS-FS, BPS-C, and BPS-N. The grey-filled distributions were only used for the field-site sub-model within the nested-scales model.

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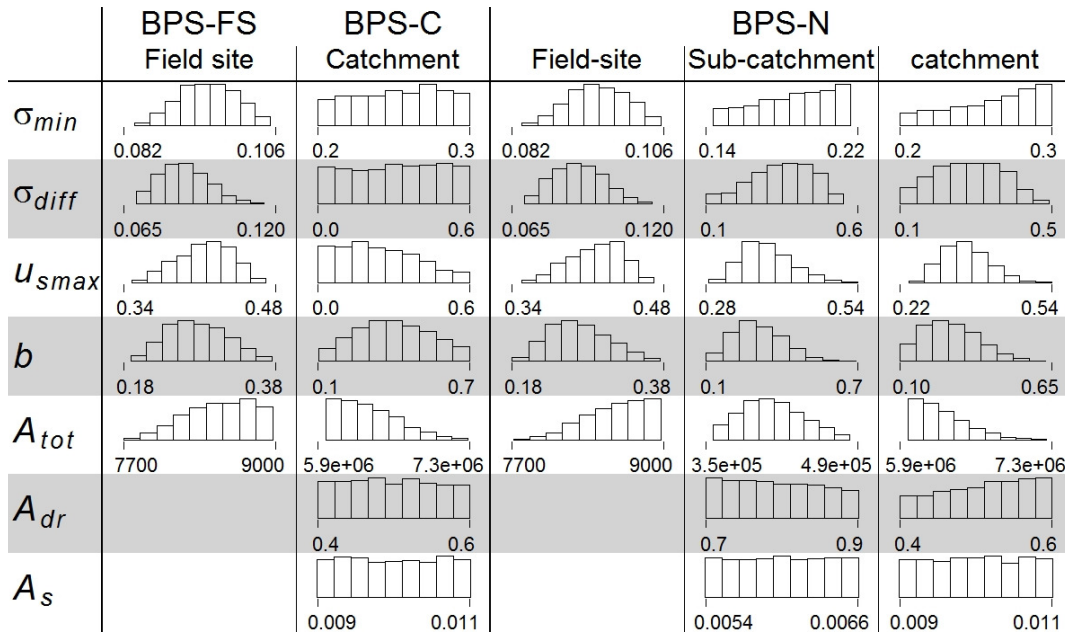


Fig. 11. Scale-specific parameter distributions for the three behavioral parameter sets: BPS-FS, BPS-C, and BPS-N.

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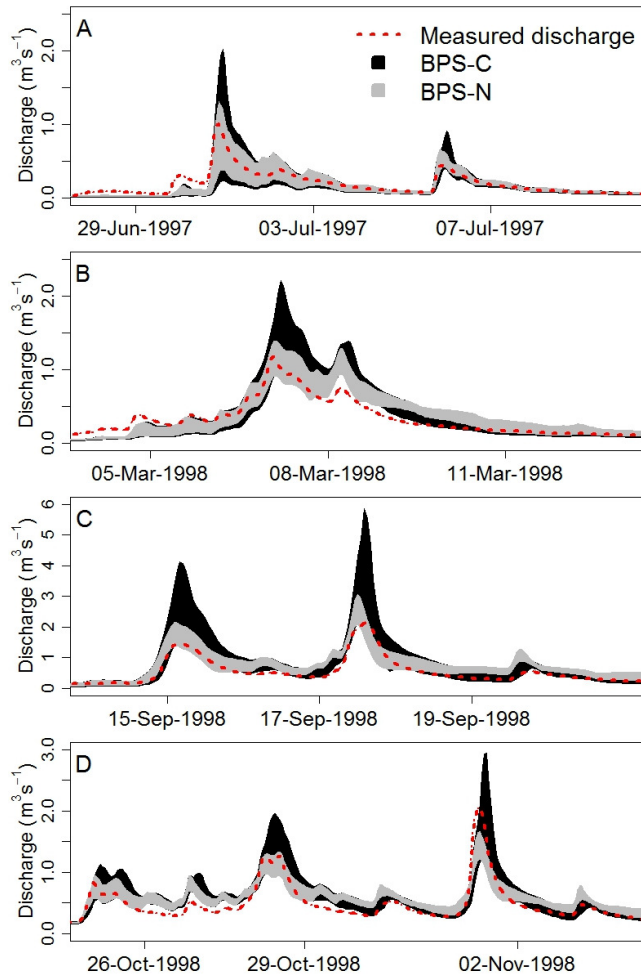


Fig. 12. Model validation results for extreme discharge events at the catchment outlet.

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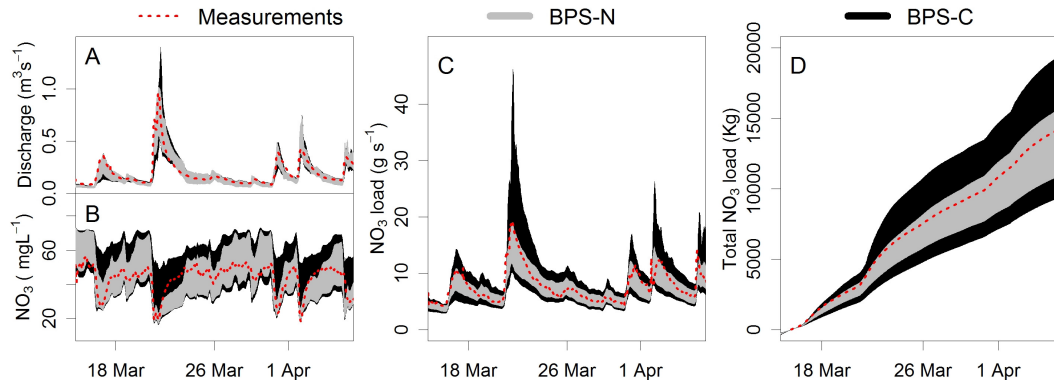


Fig. 13. Simulation results of BPS-N and BPS-C for discharge (A), nitrate concentration via a flow route mixing analysis (B), nitrate load (C) and cumulative nitrate load (D).

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