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Modelling water, sediment and nutrient fluxes from a mixed land-use catchment in New Zealand: effects of hydrologic conditions on SWAT model performance

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Abstract

The Soil Water Assessment Tool (SWAT) was configured for the Puarenga Stream catchment (77 km^2), Rotorua, New Zealand. The catchment land use is mostly plantation forest, some of which is spray-irrigated with treated wastewater. A Sequential Uncertainty Fitting (SUFI-2) procedure was used to auto-calibrate unknown parameter values in the SWAT model which was applied to the Puarenga catchment. Discharge, sediment, and nutrient variables were then partitioned into two components (base flow and quick flow) based on hydrograph separation. A manual procedure (one-at a-time sensitivity analysis) was then used to quantify parameter sensitivity for the two hydrologically-separated regimes. Comparison of simulated daily mean discharge, sediment and nutrient concentrations with high-frequency, event-based measurements allowed the error in model predictions to be quantified. This comparison highlighted the potential for model error associated with quick-flow fluxes in flashy lower-order streams to be underestimated compared with low-frequency (e.g. monthly) measurements derived predominantly from base flow measurements. To overcome this problem we advocate the use of high-frequency, event-based monitoring data during calibration and dynamic parameter values with some dependence on discharge regime. This study has important implications for quantifying uncertainty in hydrological models, particularly for studies where model simulations are used to simulate responses of stream discharge and composition to changes in irrigation and land management.

1 Introduction

Catchment models are valuable tools for understanding natural processes occurring at basin scales and for simulating the effects of different management regimes on soil and water resources (e.g. Cao et al., 2006). Model applications may have uncertainties as a result of errors associated with the forcing variables, measurements used for calibration, and conceptualisation of the model itself (Lindenschmidt et al., 2007). The

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ability of catchment models to simulate hydrological processes and pollutant loads can be assessed through analysis of uncertainty or errors during a calibration process that is specific to the application domain (White and Chaubey, 2005).

The Soil and Water Assessment Tool (SWAT) model is increasingly used to predict discharge, sediment and nutrient loads on a temporally resolved basis, and to quantify material fluxes from a catchment to the downstream receiving environment such as a lake (e.g. Nielsen et al., 2013). The SWAT model is physically-based and provides distributed descriptions of hydrologic processes at sub-basin scale (Arnold et al., 1998; Neitsch et al., 2011). It has numerous parameters, some of which can be fixed on the basis of pre-existing catchment data (e.g. soil maps) or knowledge gained in other studies. However, values for other parameters need to be assigned during a calibration process as a result of complex spatial and temporal variations that are not readily captured either through measurements or within the model algorithms themselves (Boyle et al., 2000). Such parameter values assigned during calibration are therefore lumped, i.e., they integrate variations in space and/or time and thus provide an approximation for real values which often vary widely within a study catchment. Model calibration is an iterative process whereby parameters are adjusted to the system of interest by refining model predictions to fit closely with observations under a given set of conditions (Moriasi et al., 2007). Manual calibration depends on the system used for model application, the experience of the modellers, and knowledge of the model algorithms. It tends to be subjective and time-consuming. By contrast, auto-calibration provides a less labour-intensive approach by using optimisation algorithms (Eckhardt and Arnold, 2001). The Sequential Uncertainty Fitting (SUFI-2) procedure has previously been applied to auto-calibrate discharge parameters in a SWAT application for the Thur River, Switzerland (Abbaspour et al., 2007), as well as for groundwater recharge, evapotranspiration and soil storage water considerations in West Africa (Schuol et al., 2008). Model validation is subsequently performed using measured data that are independent of those used for calibration (Moriasi et al., 2007).

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Values for hydrological parameter values in the SWAT model can vary temporally. Cibin et al. (2010) found that the optimum calibrated values for hydrological parameters varied with different flow regimes (low, medium and high), thus suggesting that SWAT model performance can be optimised by assigning parameter values based on hydrological characteristics. Other work has similarly demonstrated benefits from assigning separate parameter values to low, medium, and high discharge periods (Yilmaz et al., 2008), or based on whether a catchment is in a dry, drying, wet or wetting state (Choi and Beven, 2007). Such temporal dependence of model parameterisation on hydrologic conditions has implications for model performance. Krause et al. (2005) compared different statistical metrics of hydrological model performance separately for base-flow periods and storm events to evaluate the performance. They found that the logarithmic form of the Nash-Sutcliffe efficiency (NSE) value provided more information on the sensitivity of model performance for simulations of discharge during storm events, while the relative form of NSE was better for base flow periods. Similarly, Guse et al. (2014) investigated temporal dynamics of sensitivity of hydrological parameters and SWAT model performance using Fourier amplitude sensitivity test (Reusser et al., 2011) and cluster analysis (Reusser et al., 2009). They found that three groundwater parameters were highly sensitive during quick flow, while one evaporation parameter was most sensitive during base flow, and model performance was also found to vary significantly for the two flow regimes. Zhang et al. (2011) calibrated SWAT hydrological parameters for periods separated on the basis of six climatic indexes. Model performance improved when different values were assigned to parameters based on six hydroclimatic periods. Similarly, Pfannerstill et al. (2014) found that assessment of model performance was improved by considering an additional performance statistic for very low-flow simulations amongst five hydrologically-separated regimes.

To date, analysis of temporal dynamics of SWAT parameters has predominantly focussed on simulations of discharge rather than water quality constituents. This partly reflects the paucity of comprehensive water quality data for many catchments; near-continuous discharge data can readily be collected but this is not the case for water

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quality parameters such as suspended sediment or nutrient concentrations. Data collected in monitoring programmes that involve sampling at regular time intervals (e.g. monthly) are often used to calibrate water quality models, but these are unlikely to fully represent the range of hydrologic conditions in a catchment (Bieroza et al., 2014). In particular, water quality data collected during storm-flow periods are rarely available for SWAT calibration, thus prohibiting opportunities to investigate how parameter sensitivity varies under conditions which can contribute disproportionately to nutrient or sediment transport, particularly in lower-order catchments (Chiwa et al., 2010; Abell et al., 2013). Failure to fully consider storm-flow processes could therefore result in overestimation of model performance. Thus, further research is required to examine how water quality parameters vary during different flow regimes and to understand how model uncertainty may vary under future climatic conditions that affect discharge regimes (Brigode et al., 2013).

In this study, the SWAT model was configured to a relatively small, mixed land use catchment in New Zealand that has been the subject of an intensive water quality sampling programme designed to target a wide range of hydrologic conditions. A catchment-wide set of parameters was calibrated using the SUFI-2 procedure which is integrated into the SWAT Calibration and Uncertainty Program (SWAT-CUP). The objectives of this study were to: (1) quantify the performance of the model in simulating discharge and fluxes of suspended sediments and nutrients at the catchment outlet, (2) rigorously evaluate model performance by comparing daily simulation output with monitoring data collected under a range of hydrologic conditions; and (3) quantify whether parameter sensitivity varies between base flow and quick flow conditions.

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2 Methods

2.1 Study area and model configuration

The Puarenga Stream is the second-largest surface inflow (2.03 $m^3 s^{-1}$) to Lake Rotorua (Bay of Plenty, New Zealand) and drains a catchment of 77 km^2. The predominant land use (47 %) is exotic forest (*Pinus radiata*). Approximately 26 % is managed pastoral farmland, 11 % mixed scrub and 9 % indigenous forest. Since 1991, treated wastewater has been pumped from the Rotorua Wastewater Treatment Plant and spray-irrigated over 16 blocks of total area of 1.93 km^2 in the Whakarewarewa Forest (Fig. 1a). Following this, it took approximately four years before elevated nitrate concentrations were measured in the receiving waters of the Puarenga Stream (Lowe et al., 2007). Prior to 2002, the irrigation schedule entailed applying wastewater to two blocks per day so that each block was irrigated approximately weekly. Since 2002, 10 to 14 blocks have been irrigated simultaneously at daily frequency. Over the entire period of irrigation, nutrient concentrations in the irrigated water have gradually decreased as improvements in treatment of the wastewater have been made (Lowe et al., 2007).

Measurements from the Forest Research Institute (FRI) stream-gauge (1.7 km upstream of Lake Rotorua; Fig. 1b) were considered representative of the downstream/outlet conditions of the Puarenga Stream. The FRI stream-gauge was closed in mid 1997, then reopened late in 2004 (Environment Bay of Plenty, 2007). Discharge records during 1998–2004 were intermittent. In July 2010, the gauge was repositioned 720 m downstream to the State Highway 30 (SH 30) bridge (Fig. 1b).

SWAT input data requirements included a digital elevation model, meteorological records, records of springs and water abstraction, soil characteristics, land use classification, and management schedules for key land uses (pastoral farming, wastewater irrigation, and timber harvesting). Descriptions and sources of the data used to configure the SWAT model are given in Table 1. Values of SWAT required parameters were assigned based on: (i) measured data (e.g. most of the soil parameters; Table 1),

(ii) literature values from published studies of similar catchments (e.g. parameters for dominant land uses; Table 2); or (iii) calibrated values if other information was lacking.

2.2 Parameter calibration

Unknown parameter values (Table 3) were assigned based on either automated or manual calibration. Manual calibration was undertaken for 11 parameters related to total phosphorus (TP), while a Sequential Uncertainty Fitting (SUFI-2) procedure was applied to auto-calibrate 31 parameters for simulations of discharge and suspended sediment (SS), and 17 parameters related to total nitrogen (TN). SUFI-2 involves Latin hypercube sampling (LHS) which is a method that efficiently quantifies and constrains parameter uncertainties from default ranges with the fewest number of iterations. It generates a sample of plausible parameter values from a multidimensional distribution and is widely applied in uncertainty analysis (Marino et al., 2008). SUFI-2 considers two criteria to constrain uncertainty in each iteration. One is the P-factor, the percentage of measured data bracketed by 95 % prediction uncertainty (95PPU). Another is the R-factor, the average thickness of the 95PPU band divided by the standard deviation of measured data. Subsequent iterations were undertaken to produce narrower parameter ranges. Optimal parameter values were considered to occur when > 90 % of measured data was bracketed by simulated output and the R-factor was close to one. Spatial distribution of parameters was not considered in this study as a result of the small study area size (77 km^2). Steps in the SUFI-2 application are outlined by Abbaspour et al. (2004) who integrated the SUFI-2 procedure into the SWAT Calibration and Uncertainty program (SWAT-CUP) and linked SWAT-CUP to the SWAT model. SWAT simulates loads of "mineral phosphorus" (MINP) and "organic phosphorus" (ORGP) of which the sum is total phosphorus (TP). The MINP fraction represents soluble P either in mineral or in organic form, while ORGP refers to particulate P bound either by algae or by sediment (White et al., 2014). Soluble P may be uptaken during algae growth, or be released from benthic sediment. Either fraction can be transformed to particulate P contained in algae or sediment.

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SWAT simulates loads of nitrate-nitrogen (NO_3–N), ammonium-nitrogen (NH_4–N) and organic nitrogen (ORGN), the sum of which is total nitrogen (TN). Nitrogen parameters were auto-calibrated for each N fraction. The SWAT model does not account for the initial nitrate concentration in shallow aquifers, an issue also noted by Conan et al. (2003). Ekanayake and Davie (2005) indicated that SWAT underestimated N loading from groundwater and suggested a modification by adding a background concentration of nitrate in streamflow to represent groundwater nitrate contributions. We added 0.44 mg N L^{-1} to all model estimates of TN concentration, based on groundwater composition data from Paku (2001).

2.3 Model evaluation

Discharge measured every 15 min and water quality data collected monthly by Bay of Plenty Regional Council at the FRI stream gauge (Fig. 1b), were used for model evaluation. Daily mean discharge (from 15 min measurements) was compared with daily mean simulated discharge. Concentrations of SS, TP and TN measured monthly were compared with the respective simulated monthly values (derived from daily mean outputs). The calibration period was from 2004 to 2008 and the validation period was from 1994 to 1997. A validation period was chosen that pre-dated the calibration period because wastewater irrigation has occurred daily since 2002, compared with weekly during the validation period (1994–1997). Therefore, because the groundwater nutrient pool is not dynamically modelled in SWAT, we chose to calibrate the model to reflect current operations so that it can later be used to examine how changes to land management may affect current water quality.

In addition, high-frequency (1–2 h) water quality sampling was undertaken at the FRI stream-gauge during 2010–2012 to derive estimates of daily mean contaminant loads during storm events. Samples were analysed for SS (nine events), TP and TN (both 14 events) over sampling periods of 24–73 h. The sampling programme was designed to encompass pre-event base flow, storm generated quick flow and post-event base flow (Abell et al., 2013). These data permitted calculation of daily discharge-weighted (*Q*-

weighted) mean concentrations to compare with modelled daily mean estimates. The Q-weighted mean concentrations C_{QWM} were calculated as:

$$C_{\mathrm{QWM}} = \frac{\sum_{i=1}^{n} C_i Q_i}{\sum_{i=1}^{n} Q_i} \tag{1}$$

where n is number of samples, C_i is contaminant concentration measured at time i, and Q_i is discharge measured at time i.

Model goodness-of-fit was assessed graphically and quantified using coefficient of determination (R^2), Nash-Sutcliffe efficiency (NSE) and percent bias (PBIAS; Table 4). R^2 (range 0 to 1) and NSE (range $-\infty$ to 1) values are commonly used to evaluate SWAT model performance at daily time step (Gassman et al., 2007). PBIAS value indicates the average tendency of simulated outputs to be larger or smaller than observations (Gupta et al., 1999).

2.4 Hydrograph and contaminant load separation

The Web-based Hydrograph Analysis Tool (Lim et al., 2005) was applied to partition both measured and simulated discharges into base flow (Q_{b}) and quick flow (Q_{q}). An Eckhardt filter parameter of 0.98 and ratio of base flow to total discharge of 0.8 were assumed (cf. Lim et al., 2005). There were a total of 60 days without quick flow during the calibration period (2004–2008) and 1379 days for which hydrograph separation defined both base flow and quick flow.

Contaminant (SS, TP and TN) concentrations (C_{sep}) were partitioned into base flow (C'_{b}) and quick flow components (C'_{q}; cf. Rimmer and Hartmann, 2014) to separately examine the sensitivity of water quality parameters during base flow and quick flow:

$$C_{\mathrm{sep}} = \frac{Q_{\mathrm{q}} \times C'_{\mathrm{q}} + Q_{\mathrm{b}} \times C'_{\mathrm{b}}}{Q_{\mathrm{q}} + Q_{\mathrm{b}}} \tag{2}$$

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C'_b for each contaminant was estimated as the average concentration for the 60 days with no quick flow. C'_q for each contaminant was calculated by rearranging Eq. (2) as:

$$C'_q = \frac{(Q_q + Q_b) \times C_{sep} - Q_b \times C'_b}{Q_q} \quad (3)$$

To retain Eq. (3) rational, C'_q must be positive, therefore C'_b is the minimum between $\overline{C_{sep}}$ and C_{sep}. Measured and simulated base flow and quick flow contaminant loads were then calculated.

2.5 Sensitivity analysis

A one-at a-time (OAT) routine proposed by Morris (1991) was applied to investigate how parameter sensitivity varied between the two flow regimes (base flow and quick flow). OAT sensitivity analysis was employed by varying the parameter of interest among ten equidistant values within the default range. The standard deviation of $\log_{10}$-transformed NSE values was calculated from the sensitivity analysis for each variable and for the two flow regimes (base flow and quick flow). Parameters were ranked from most to least sensitive on the basis of the sensitivity metric (standard deviation of $\log_{10}$-transformed NSE), using a value of 0.1 as a threshold above which parameters were deemed particularly "sensitive". Methods used to quantify parameter sensitivity are illustrated in Fig. 2.

3 Results

3.1 Model performance

Modelled and measured base flow showed high correspondence, although measured daily mean discharge during storm peaks was often underestimated (Fig. 3a and e).

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Modelled SS concentrations overestimated measurements of monthly grab samples by an average of 18.3 % during calibration and 0.32 % during validation (Fig. 3b and f). Measured TP concentrations in monthly grab samples were underestimated by 23.8 % during calibration (Fig. 3c) and 24.5 % during validation (Fig. 3g). Similarly, measured TP loads were underestimated by 34.5 and 38.4 %, during calibration and validation, respectively. Modelled and measured TN concentrations were generally better aligned during base flow (Fig. 3d), apart from a mismatch prior to 1996 when monthly measured TN concentrations were substantially lower than model predictions although they gradually increased (Fig. 3h) during the validation period (1994–1997). The average measured TN load increased from 134 kg N d^{-1} prior to 1996, to 190 kg N d^{-1} post 1996. The comparable increase in modelled TN load was 167 to 205 kg N d^{-1}, respectively.

Statistical evaluations of goodness-of-fit are shown in Table 5. The R^2 values for discharge were 0.77 for calibration and 0.68 for validation, corresponding to model performance ratings of "very good" and "good" (cf. Table 4). Similarly, the NSE values for discharge were 0.73 (good) for calibration and 0.62 (satisfactory) for validation. Positive PBIAS (7.8 % for calibration and 8.8 % for validation) indicated a tendency for underestimation of daily mean discharge, however, the low magnitude of PBIAS values corresponded to a performance rating of "very good". The R^2 values for SS were 0.42 (unsatisfactory) for calibration and 0.80 for validation (very good). Similarly, the NSE values for SS were −0.08 (unsatisfactory) for calibration and 0.76 (very good) for validation. The model did not simulate trends well for monthly measured TP and TN concentrations. The R^2 values for TP and TN were both < 0.1 (unsatisfactory) during calibration and validation and NSE values were both < 0 (unsatisfactory). Values of PBIAS corresponded to "good" or "very good" performance ratings for TP and TN.

Observed Q-weighted daily mean concentrations derived from hourly measurements and simulated daily mean concentrations of SS, TP and TN during an example two-day storm event are shown in Fig. 4a–c. The simulation of SS and TN concentrations was somewhat better than for TP. Comparisons of Q-weighted daily mean concentrations

(C_{QWM}) during storm events from 2010 to 2012 are shown in Fig. 4d–f for SS (nine events), TP and TN (both 14 events). The C_{QWM} of TP exceeded the simulated daily mean by between 0.02 and 0.2 mg P L^{-1}, and on average, the model underestimated measurements by 69.4 % (Fig. 4e). Although R^2 and NSE values for C_{QWM} of TN were unsatisfactory (Table 5), they were both close to the threshold for satisfactory performance (0.5). For C_{QWM} of SS and TP, R^2 and NSE values indicated that the model performance was unsatisfactory. The PBIAS value of −0.87 for C_{QWM} of TN corresponded to model performance ratings of "very good", while the PBIAS values for C_{QWM} of SS and TP were 43.9 and 69.4, respectively, indicating satisfactory model performance.

3.2 Parameter sensitivity

Measured and simulated discharge and contaminant concentrations for the two flow regimes (base flow and quick flow), are shown in Fig. 5. The OAT sensitivity analysis undertaken separately for base flow and quick flow identified three parameters that most influenced the quick flow estimates, and five parameters that most influenced the base flow estimates (parameters above the dashed line in Fig. 6a). Those sensitive flow parameters specifically relate to the relevant flow components, providing a mechanistic basis for the finding that they were particularly sensitive. Channel hydraulic conductivity (CH_K2) is used to estimate the peak runoff rate (Lane, 1983). Lateral flow slope length (SLSOIL) and lateral flow travel time (LAT_TIME) have an important controlling effect on the amount of lateral flow entering the stream reach during quick flow. Both slope (HRU_SLP) and soil available water content (SOL_AWC) were particularly sensitive for the base flow simulation because they affect lateral flow within the kinematic storage model in SWAT (Sloan and Moore, 1984). The aquifer percolation coefficient (RCHRG_DP) and the base flow alpha factor (ALPHA_BF) strongly influenced base flow calculations (Sangrey et al., 1984), as did the channel Manning's N value (CH_N2) which is used to estimate channel flow (Chow, 2008).

For SS loads, 12 and four parameters, respectively, were identified as sensitive in relation to the simulations of base flow and quick flow (parameters above the dashed line

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in Fig. 6b). Parameters that control main channel processes (e.g. CH_K2 and CH_N2) and subsurface water transport processes (e.g. LAT_TIME and SLSOIL) were found to be much more sensitive for base flow SS load estimations. Exclusive parameters for SS estimations, such as SPCON (linear parameter), PRF (peak rate adjustment factor), SPEXP (exponent parameter), CH_COV1 (channel erodibility factor), and CH_COV2 (channel cover factor) were found to be much more sensitive in base flow SS load, while LAT_SED (SS concentration in lateral flow and groundwater flow) was more sensitive in quick flow SS load. Parameters that control overland processes, e.g. CN2 (the curve number), OV_N (overland flow Manning's *N* value) and SLSUBBSN (sub-basin slope length), were found to be much more sensitive for quick flow SS load estimations.

Of the sensitive parameters, BC4 (ORGP mineralization rate) was particularly sensitive for the simulation of base flow MINP load (Fig. 6c). RCN (nitrogen concentration in rainfall) related specifically to the dynamics of the base flow NO_3–N load and NPERCO (nitrogen percolation coefficient) significantly affected quick flow NO_3–N load (Fig. 6d). Parameter CH_ONCO (channel ORGN concentration) similarly affected both flow components of ORGN load (Fig. 6e) and SOL_CBN (organic carbon content) was most sensitive for the simulations of quick flow ORGN and NH_4–N loads. Parameter BC1 (nitrification rate in reach) was particularly sensitive for the simulation of base flow NH_4–N load (Fig. 6f).

4 Discussion

4.1 Temporal dynamics of model performance

This study examined temporal dynamics of model performance and parameter sensitivity in a SWAT model application that was configured for a small, relatively steep and lower order stream catchment in New Zealand. This country faces increasing pressures on freshwater resources (Parliamentary Commissioner for the Environment, 2013) and models such as SWAT potentially offer valuable tools to inform management of water resources although, to date, the SWAT model has received limited consideration in New Zealand (Cao et al., 2006). Model evaluation on the basis of the data collected during an extended monitoring programme enabled a detailed examination of how model performance varied during different flow regimes. It also permitted error in daily mean estimates of contaminant loads to be quantified with relative precision, allowing assessment of the ability of SWAT model to simulate contaminant loads during storm events when lower-order streams typically exhibit considerable sub-daily variability in both discharge and contaminant concentrations (Zhang et al., 2010). Separating discharge and loads of sediments and nutrients into those associated with base flow and quick flow for separate OAT sensitivity analyses provided important insights into the varying dependency of parameter sensitivity on hydrologic conditions.

The poor fit between simulated daily mean TP concentrations and monthly instantaneous measurements may partly reflect a mismatch between the dominant processes affecting phosphorus cycling in the stream and those represented in SWAT. The ORGP fraction that is simulated in SWAT includes both organic and inorganic forms of particulate phosphorus, however, the representation of particulate phosphorus cycling only focusses on organic phosphorus cycling with limited consideration of interactions between inorganic streambed sediments and dissolved reactive phosphorus in overlying water (White et al., 2014). This contrasts with phosphorus cycling in the study stream where it has been shown that dynamic sorption processes between the dissolved and particulate inorganic phosphorus pools exert major control on phosphorus cycling (Abell and Hamilton, 2013).

Overestimation of TN concentration prior to 1996 (PBIAS = −26.7 %) reflects the fact that NO_3–N concentrations in groundwater were likely higher during the calibration period (PBIAS = −0.05 %; 2004–2008) due to wastewater irrigation operations, and had reached a new quasi-steady state between wastewater loads and in-stream attenuation. Our decision to deliberately select a validation period (1994–1997) during which the boundary conditions of system (anthropogenic nutrient loading) differed considerably from the calibration period allowed us to rigorously assess the capability of SWAT

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to accurately predict water quality under an altered management scenario (i.e. the purpose of most SWAT applications). Our results also highlight a discrepancy between the static nature of the groundwater nitrogen pool represented in SWAT and the reality that groundwater nutrient concentrations change dynamically in a lagged response to changes to sources in modified catchments (Bain et al., 2012).

Our finding that measured Q-weighted mean concentrations (C_{QWM}) of TP and SS during storm events (2010–2012) were greatly underestimated relative to simulated daily mean TP (PBIAS = 69.4 %) and SS (PBIAS = 43.9 %) concentrations has important implications for studies that examine effects of altered flow regimes on contaminant transport. For example, studies which simulate scenarios comprising more frequent large rainfall events (associated with climate change predictions for many regions; IPCC, 2013) may considerably underestimate projected future loads of SS and associated particulate nutrients if only base flow water quality measurements (i.e. those predominantly collected during "state of environment" monitoring) are used for calibration/validation (see Radcliffe et al., 2009 for a discussion of this issue in relation to phosphorus). This is also reflected by the two model performance statistics relating to validation of modelled SS concentrations using monthly grab samples (predominantly base flow; "very good") and C_{QWM} estimated during storm sampling ("unsatisfactory") based on R^2 and NSE values. Furthermore, the disparity in goodness-of-fit statistics between discharge (typically "good" or "very good") and nutrient variables (often "unsatisfactory") highlights the potential for catchment models which inadequately represent contaminant cycling processes (manifest in unsatisfactory concentration estimates) to nevertheless produce satisfactorily load predictions. This highlights the potential for model uncertainty to be underestimated in studies which aim to predict the effects of scenarios associated with changes in contaminant cycling such as increases in fertiliser application rates.

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4.2 Temporal dynamics of parameter sensitivity

To date, studies of temporal variability of parameters have focused on hydrological parameters, rather than on water quality parameters. Defining separate contaminant concentrations in base flow and quick flow enabled us to examine how the sensitivity of water quality parameters varied depending on hydrologic conditions.

In a study of a lowland catchment (481 km^2), Guse et al. (2014) found that three groundwater parameters, RCHRG_DP (aquifer percolation coefficient), GW_DELAY (groundwater delay) and ALPHA_BF (base flow alpha factor) were highly sensitive in relation to simulating discharge during quick flow, while ESCO (soil evaporation compensation factor) was most sensitive during base flow. This is counter to the findings of this study for which the base-flow discharge simulation was sensitive to RCHRG_DP and ALPHA_BF. This result may reflect that, relative to our study catchment, the catchment studied by Guse et al. (2014) had moderate precipitation (884 $mm\,y^{-1}$) with less forest cover and flatter topography. Although the GW_DELAY parameter reflects the time lag that it takes water in the soil water to enter the shallow aquifers, its lack of sensitivity under both base flow and quick flow conditions in this study is a reflection of higher water infiltration rates and steeper slopes. The ESCO parameter controls the upwards movement of water from lower soil layers to meet evaporative demand (Neitsch et al., 2011). Its lack of sensitivity in our study may reflect relatively high and seasonally-consistent rainfall (1500 $mm\,y^{-1}$), in addition to extensive forest cover in the Puarenga Stream catchment, which reduces soil evaporative demand by shading. Soil texture is also likely a contributor to this result. The predominant soil horizon type in the Puarenga Stream catchment was A, indicating high macroporosity which promotes high water infiltration rate and inhibits upward transport of water by capillary action (Neitsch et al., 2011). The variability in the sensitivity of the parameter SURLAG (surface runoff lag coefficient) between this study (relatively insensitive) and that of Cibin et al. (2010; relatively sensitive) likely reflects differences in catchment size. The Puarenga Stream catchment (77 km^2) is much smaller than the study catchment (St

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Joseph River; 2800 km^2) of Cibin et al. (2010) and, consequently, distances to the main channel are much shorter, with less potential for attenuation of surface runoff in off-channel storage sites. The curve number (CN2) parameter was not found to be sensitive in both this study and Shen et al. (2012), because surface runoff was simulated based on the Green and Ampt method (1911) requiring the hourly rainfall inputs, rather than the curve number equation which is an empirical model. By contrast, the most sensitive parameters in our study are those that determine the extent of lateral flow, an important contributor to streamflow in the catchment, due to a general lack of ground cover under plantation trees and formation of gully networks on steep terrain.

Parameters that control surface water transport processes (e.g. LAT_TIME and SLSOIL) were found to be much more sensitive for base flow SS load estimation than parameters that control groundwater processes (e.g. ALPHA_BF and RCHRG_DP), reflecting the importance of surface flow processes for sediment transport. Sensitive parameters for quick flow SS load estimation related to overland flow processes (e.g. OV_N and SLSUBBSN), thus reflecting the fact that sediment transport is largely dependent on rainfall-driven processes, as is typical of steep and lower-order catchments. Modelled base flow NO_3–N loads were most sensitive to the nitrogen concentration in rainfall (RCN) because of rainfall as a predominant contributor to recharging base flow. The nitrogen percolation coefficient (NPERCO) was more influential for quick flow NO_3–N load estimation, probably indicating that the quick flow NO_3–N load is more influenced by the mobilisation of concentrated nitrogen sources associated with agriculture or treated wastewater distribution. High sensitivity of the organic carbon content (SOL_CBN) for quick flow ORGN load estimates likely reflects mobilisation of N associated with organic material following rainfall. The finding that base flow NH_4–N load was more sensitive to nitrification rate in reach (BC1) likely reflects that base flow provides more favourable conditions to complete this oxidation reaction, as NH_4–N is less readily leached and transported. Similarly, the ORGP mineralization rate (BC4) strongly influenced base flow MINP load estimation, reflecting that base flow phosphorus transport is relatively more influenced by cycling from channel bed stores, whereas

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quick flow phosphorus transport predominantly reflects the transport of phosphorus that originated from sources distant from the channel.

5 Conclusions

The performance of a SWAT model was quantified for different hydrologic conditions in a small catchment with mixed land use. Discharge-weighted mean concentrations of TP and SS measured during storm events were greatly underestimated by SWAT, highlighting the potential for uncertainty to be greatly underestimated in catchment model applications that are validated using a sample of contaminant load measurements that is over-represented by measurements made during base flow conditions. Accurate simulation of nitrogen concentrations was constrained by the non-steady state of groundwater nitrogen concentrations due to historic variability in anthropogenic nitrogen applications to land. The sensitivity of many parameters varied depending on the relative dominance of base flow and quick flow, while curve number, soil evaporation compensation factor, surface runoff lag coefficient, and groundwater delay were largely invariant to the two flow regimes. Parameters relating to main channel processes were more sensitive when estimating variables during base flow, while those relating to overland processes were more sensitive for quick flow. Temporal dynamics of both parameter sensitivity and model performance due to dependence on hydrologic conditions should be considered in further model applications. Monitoring programmes which collect high-frequency and event-based data have an important role in supporting the robust calibration and validation of SWAT model applications.

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Table 1. Description of data used to configure and calibrate the SWAT model.

Data	Application	Data description and configuration details	Source
Digital elevation model (DEM) and digitized stream network	Sub-basin delineation (Fig. 1b)	25 m resolution. Used to define five slope classes: 0–4 %, 4–10 %, 10–17 %, 17–26 % and > 26 %.	Bay of Plenty Regional Council (BoPRC)
Stream discharge and water quality measurements	Calibration (2004–2008) and validation (1994–1997; 2010–2012)	FRI: 15–min stream discharge (1994–1997; 2004–2008), monthly grab samples for instantaneous SS, TP and TN concentrations (1994–1997; 2004–2008), high–frequency event–based samples for concentrations of SS (nine events), TP and TN (both 14 events) at 1–2 h frequency (2010–2012).	BoPRC; Abell et al. (2013)
Spring discharge, nutrient loads, and water abstraction volumes	Point source (Fig. 1b) and water use	Constant daily discharge assigned to two cold-water springs (Waipa Spring and Hemo Spring) and one geothermal spring based on spot measurements. Constant nutrient concentrations assigned to Waipa Spring and Hemo Spring and the geothermal spring based on samples collected between Aug 1984 and Jun 2004. Monthly water abstraction assigned to two cold-water springs.	Kusabs and Shaw (2008); White et al. (2004); Proffit (2009) (Unpublished Site Visit Report); Paku (2001); Mahon (1985); Glover (1993); Jowett (2008); Rotorua District Council (personal communication, 2012)
Land use	HRU definition	25 m resolution, 10 basic land-cover categories. Some particular land-cover parameters were prior-estimated (Table 2).	New Zealand Land Cover Database Version 2; BoPRC
Soil characteristics	HRU definition	Properties of 22 soil types were determined using the key physical properties and the characteristics of functional horizons provided by soil map.	New Zealand Land Resource Inventory and digital soil map (available at http://smap.landcareresearch.co.nz)

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Table 1. Continued.

Data	Application	Data description and configuration details	Source
Meteorological data	Meteorological forcing	Daily maximum and minimum temperature, daily mean relative humidity, daily global solar radiation, daily (9 a.m.) surface wind speed and hourly precipitation.	National Climatic Data Centre (available at http://cliflo.niwa.co.nz/); Kaituna rain gauge (Fig. 1a)
Agricultural management practices	Agricultural management schedules	Farm-specific stocking density, fertilizer application rates and farming practices (1993–2012). Simulated applications of urea (twice in winter/spring; four times in summer/autumn) and di-ammonium phosphate (once or twice in spring/autumn). Application of manure-associated nutrients to paddocks was simulated as a function of stock numbers and literature values for the average N and P content of excreta.	Statistics New Zealand (2006); Fert Research (2009); Ledgard and Thorrold (1998); Dairying Research Corporation (1999)
Nutrient loading by wastewater application	Nonpoint-source from land treatment irrigation	Wastewater application rates and effluent composition (TN and TP concentration) for 16 spray blocks from 1996–2012. Each spray block was assigned an individual management schedule specifying daily application rates.	Rotorua District Council (2006)
Forest stand map and harvest dates	Forestry planting and harvesting operations	Planting and harvesting data for 472 ha forestry stands. Prior to 2007 we assumed stands were cleared one-year prior to the establishment year. Post 2007, harvesting date was assigned to the first day of harvesting month.	Timberlands Limited, Rotorua, New Zealand (personal communication, 2012)

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Table 2. Prior-estimated parameter values for three dominant types of land-cover in the Puarenga Stream catchment. Values of other land use parameters were based on the default values in the SWAT database.

Land-cover type	Parameter	Definition	Value	Source
PINE (*Pinus radiata*)	HVSTI	Percentage of biomass harvested	0.65	(Ximenes et al., 2008)
	T_OPT (°C)	Optimal temperature for plant growth	15	(Kirschbaum and Watt, 2011)
	T_BASE (°C)	Minimum temperature for plant growth	4	(Kirschbaum and Watt, 2011)
	MAT_YRS	Number of years to reach full development	30	(Kirschbaum and Watt, 2011)
	BMX_TREES (tonnes ha^{-1})	Maximum biomass for a forest	400	(Bi et al., 2010)
	GSI ($m\,s^{-1}$)	Maximum stomatal conductance	0.00198	(Whitehead et al., 1994)
	BLAI ($m^2\,m^{-2}$)	Maximum leaf area index	5.2	(Watt et al., 2008)
	BP3	Proportion of P in biomass at maturity	0.000163	(Hopmans and Elms, 2009)
	BN3	Proportion of N in biomass at maturity	0.00139	(Hopmans and Elms, 2009)
FRSE (Evergreen forest)	HVSTI	Percentage of biomass harvested		–
	BMX_TREES (tonnes ha^{-1})	Maximum biomass for a forest	372	(Hall et al., 2001)
	MAT_YRS (years)	Number of years for tree to reach full development	100	–
PAST (Pastoral farm)	T_OPT (°C)	Optimal temperature for plant growth	25	(McKenzie et al., 1999)
	T_BASE (°C)	Minimum temperature for plant growth	5	(McKenzie et al., 1999)

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Table 3. Summary of calibrated SWAT parameters. Discharge (*Q*), suspended sediment (SS) and total nitrogen (TN) parameter values were assigned using auto-calibration, while total phosphorus (TP) parameters were manually calibrated. SWAT default ranges and input file extensions are shown for each parameter.

Parameter	Definition	Unit	Default range
Q and SS			
EVRCH.bsn	Reach evaporation adjustment factor		0.5–1
PRF.bsn	Peak rate adjustment factor for sediment routing in the main channel		0–2
SPCON.bsn	Linear parameter for calculating the maximum amount of sediment that can be re-entrained during channel sediment routine		0.0001–0.01
SPEXP.bsn	Exponent parameter for calculating sediment re-entrained in channel sediment routine		1–1.5
SURLAG.bsn	Surface runoff lag coefficient		0.05–24
ALPHA_BF.gw	Base flow alpha factor (0–1)		0.0071–0.0161
GW_DELAY.gw	Groundwater delay		0–500
GW_REVAP.gw	Groundwater “revap” coefficient		0.02–0.2
GW_SPYLD.gw	Special yield of the shallow aquifer	$m^3 m^{-3}$	0–0.4
GWHT.gw	Initial groundwater height		0–25
GWQMN.gw	Threshold depth of water in the shallow aquifer required for return flow to occur	mm	0–5000
RCHRG_DP.gw	Deep aquifer percolation fraction		0–1
REVAPMN.gw	Threshold depth of water in the shallow aquifer required for “revap” to occur	mm	0–500
CANMX. hru	Maximum canopy storage	mm	0–100
EPCO. hru	Plant uptake compensation factor		0–1
ESCO. hru	Soil evaporation compensation factor		0–1
HRU_SLP. hru	Average slope steepness	m m – 1	0–0.6
LAT_SED. hru	Sediment concentration in lateral flow and groundwater flow	$mg L^{-1}$	0–5000
LAT_TTIME. hru	Lateral flow travel time		0–1800
OV_N. hru	Manning’s *N* value for overland flow		0.01–30
RSDIN. hru	Initial residue cover	kg ha – 1	0–10 000
SLSOIL. hru	Slope length for lateral subsurface flow		0–150
SLSUBBSN. hru	Average slope length		10–150
CH_COV1.rte	Channel erodibility factor		0–0.6
CH_COV2.rte	Channel cover factor		0–1
CH_K2.rte	Effective hydraulic conductivity in the main channel alluvium	$mm h^{-1}$	0–500
CH_N2.rte	Manning’s *N* value for the main channel		0–0.3
CH_K1.sub	Effective hydraulic conductivity in the tributary channel alluvium	$mm h^{-1}$	0–300
CH_N1.sub	Manning’s *N* value for the tributary channel		0.01–30
CN2. mgt	Initial SCS runoff curve number for moisture condition		35–89
USLE_P.mgt	USLE equation support practice factor		0–1

Table 3. Continued.

Parameter	Definition	Unit	Default range
TP			
P_UPDIS.bsn	Phosphorus uptake distribution parameter		0–100
PHOSKD.bsn	Phosphorus soil partitioning coefficient		100–200
PPERCO.bsn	Phosphorus percolation coefficient		10–17.5
PSP.bsn	Phosphorus sorption coefficient		0.01–0.7
GWSOLP.gw	Soluble phosphorus concentration in groundwater loading	$mg\,P\,L^{-1}$	0–1000
LAT_ORGP.gw	Organic phosphorus in the base flow	$mg\,P\,L^{-}$	0–200
ERORGP. hru	Organic phosphorus enrichment ratio		0–5
CH_OPCO.rte	Organic phosphorus concentration in the channel	$mg\,P\,L^{-1}$	0–100
BC4.swq	Rate constant for mineralization of organic phosphorus to dissolved phosphorus in the reach at 20 °C	d^{-1}	0.01–0.7
RS2.swq	Benthic (sediment) source rate for dissolved phosphorus in the reach at 20 °C	$mg\,m^{-2}\,d^{-1}$	0.001–0.1
RS5.swq	Organic phosphorus settling rate in the reach at 20 °C	d^{-1}	0.001–0.1
TN			
RSDCO.bsn	Residue decomposition coefficient		0.02–0.1
CDN.bsn	Denitrification exponential rate coefficient		0–3
CMN.bsn	Rate factor for humus mineralization of active organic nitrogen		0.001–0.003
N_UPDIS.bsn	Nitrogen uptake distribution parameter		0–100
NPERCO.bsn	Nitrogen percolation coefficient		0–1
RCN.bsn	Concentration of nitrogen in rainfall	$mg\,N\,L^{-1}$	0–15
SDNCO.bsn	Denitrification threshold water content		0–1
HLIFE_NGW.gw	Half-life of nitrat-nitrogen in the shallow aquifer	d^{-1}	0–200
LAT_ORGN.gw	Organic nitrogen in the base flow	$mg\,N\,L^{-1}$	0–200
SHALLST_N.gw	Nitrat-nitrogen concentration in the shallow aquifer	$mg\,N\,L^{-1}$	0–1000
ERORGN. hru	Organic nitrogen enrichment ratio		0–5
CH_ONCO.rte	Organic nitrogen concentration in the channel	$mg\,N\,L^{-1}$	0–100
BC1.swq	Rate constant for biological oxidation of ammonium–nitrogen to nitrit–nitrogen in the reach at 20 °C	d^{-1}	0.1–1
BC2.swq	Rate constant for biological oxidation of nitrit–nitrogen to nitrat–nitrogen in the reach at 20 °C	d^{-1}	0.2–2
BC3.swq	Rate constant for hydrolysis of organic nitrogen to ammonium–nitrogen in the reach at 20 °C	d^{-1}	0.2–0.4
RS3.swq	Benthic (sediment) source rate for ammonium–nitrogen in the reach at 20 °C	$mg\,m^{-2}\,d^{-1}$	0–1
RS4.swq	Rate coefficient for organic nitrogen settling in the reach at 20 °C	d^{-1}	0.001–0.1

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Table 4. Criteria for model performance. Note: o_n is the nth observed datum, s_n is the nth simulated datum, $\overline{o}$ is the observed mean value, $\overline{s}$ is the simulated daily mean value, and N is the total number of observed data. Performance rating criteria are based on Moriasi et al. (2007) for Q: discharge, SS: suspended sediment, TP: total phosphorus and TN: total nitrogen.

Statistic equation	Constituent	Performance ratings			
		Unsatisfactory	Satisfactory	Good	Very good
$R^2 = \frac{\left(\sum_{n=1}^{N}\left((s_n-\bar{s})(o_n-\bar{o})\right)\right)^2}{\sum_{n=1}^{N}(o_n-\bar{o})^2 \times \sum_{n=1}^{N}(s_n-\bar{s})^2}$ (2)	All	< 0.5	0.5–0.6	0.6–0.7	0.7–1
$\text{NSE} = 1 - \frac{\sum_{n=1}^{N}(o_n-s_n)^i}{\sum_{n=1}^{N}(o_n-\bar{o})^i}$ $i = 2$ (3)	All	< 0.5	0.5–0.65	0.65–0.75	0.75–1
$\pm\text{PBIAS}\,\% = \frac{\sum_{n=1}^{N}(o_n-s_n)}{\sum_{n=1}^{N}o_n} \times 100$ (4)	Q	> 25	15–25	10–15	< 10
	SS	> 55	30–55	15–30	< 15
	TP, TN	> 70	40–70	25–40	< 25

R^2: coefficient of determination.
NSE: Nash–Sutcliffe efficiency.
PBIAS: percent bias.

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Table 5. Model performance ratings for discharge (Q), suspended sediment (SS), total phosphorus (TP) and total nitrogen (TN) simulations. n indicates the number of measurements. Q-weighted mean concentrations were calculated using Eq. (1).

Model performance	Statistics	Q	SS	TP	TN
Calibration with		$n = 1439$	$n = 43$	$n = 45$	$n = 39$
instantaneous measurements	R^2	0.77 (Very good)	0.42 (Unsatisfactory)	0.02 (Unsatisfactory)	0.08 (Unsatisfactory)
(2004–2008)	NSE	0.73 (Good)	−0.08 (Unsatisfactory)	−1.31 (Unsatisfactory)	−0.30 (Unsatisfactory)
	±PBIAS %	7.8 (Very good)	−18.3 (Very good)	23.8 (Very good)	−0.05 (Very good)
Validation with		$n = 1294$	$n = 37$	$n = 37$	$n = 36$
instantaneous measurements	R^2	0.68 (Good)	0.80 (Very good)	0.01 (Unsatisfactory)	0.01 (Unsatisfactory)
(1994–1997)	NSE	0.62 (Satisfactory)	0.76 (Very good)	−0.97 (Unsatisfactory)	−2.67 (Unsatisfactory)
	±PBIAS %	8.8 (Very good)	−0.32 (Very good)	24.5 (Very good)	−26.7 (Good)
Validation with		–	$n = 12$	$n = 18$	$n = 18$
Q-weighted mean concentrations	R^2	–	0.38 (Unsatisfactory)	0.06 (Unsatisfactory)	0.46 (Unsatisfactory)
(2010–2012)	NSE	–	−0.03 (Unsatisfactory)	−4.88 (Unsatisfactory)	0.42 (Unsatisfactory)
	± PBIAS %	–	43.9 (Satisfactory)	69.4 (Satisfactory)	−0.87 (Very good)

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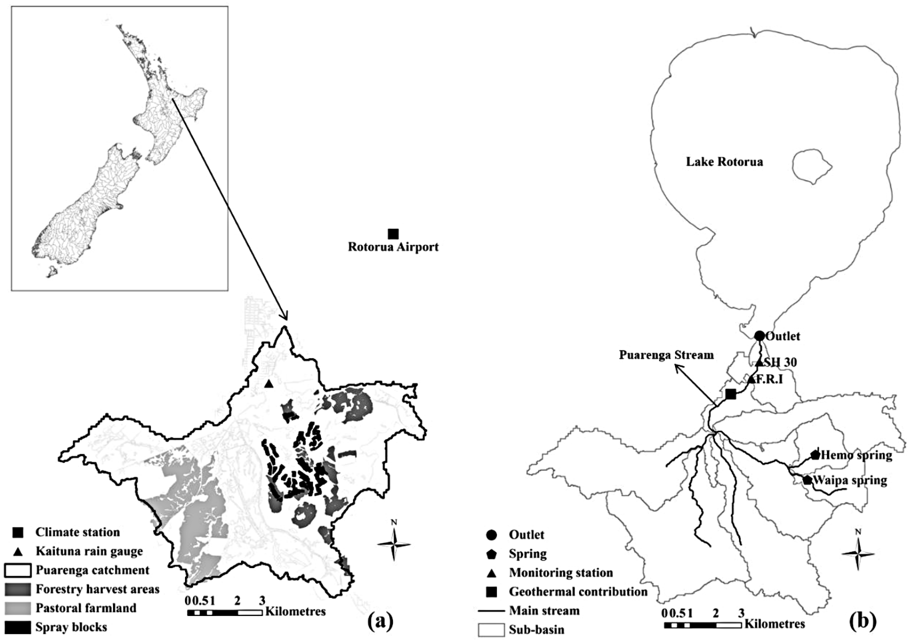

Figure 1. (a) Location of Puarenga Stream surface catchment in New Zealand, Kaituna rain gauge, climate station and managed land areas for which management schedules were prescribed in SWAT, and **(b)** location of the Puarenga Stream, major tributaries, monitoring stream-gauges, two cold-water springs and the Whakarewarewa geothermal contribution.

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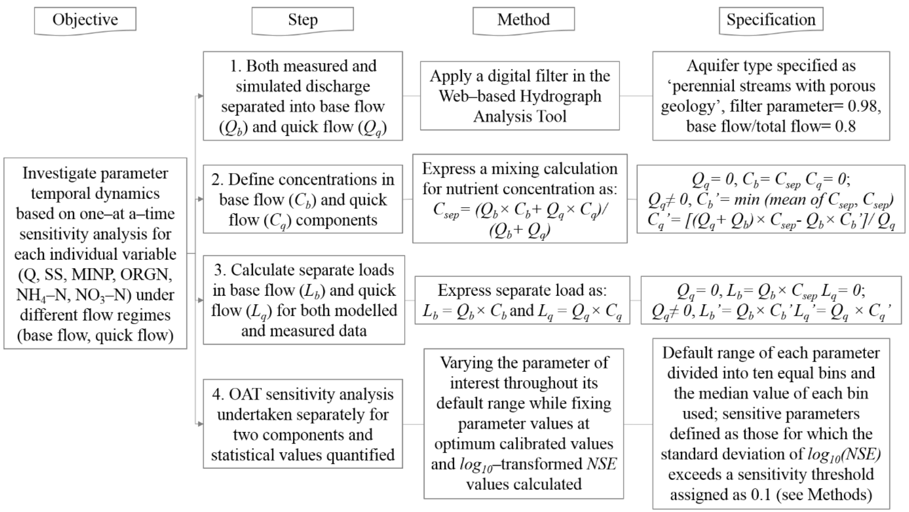

Figure 2. Flow chart of methods used for parameter sensitivity analysis in sequence of each individual variable: Q (discharge), SS (suspended sediment), MINP (mineral phosphorus), ORGN (organic nitrogen), NH_4–N (ammonium–nitrogen), and NO_3–N (nitrate–nitrogen). NSE: Nash–Sutcliffe efficiency.

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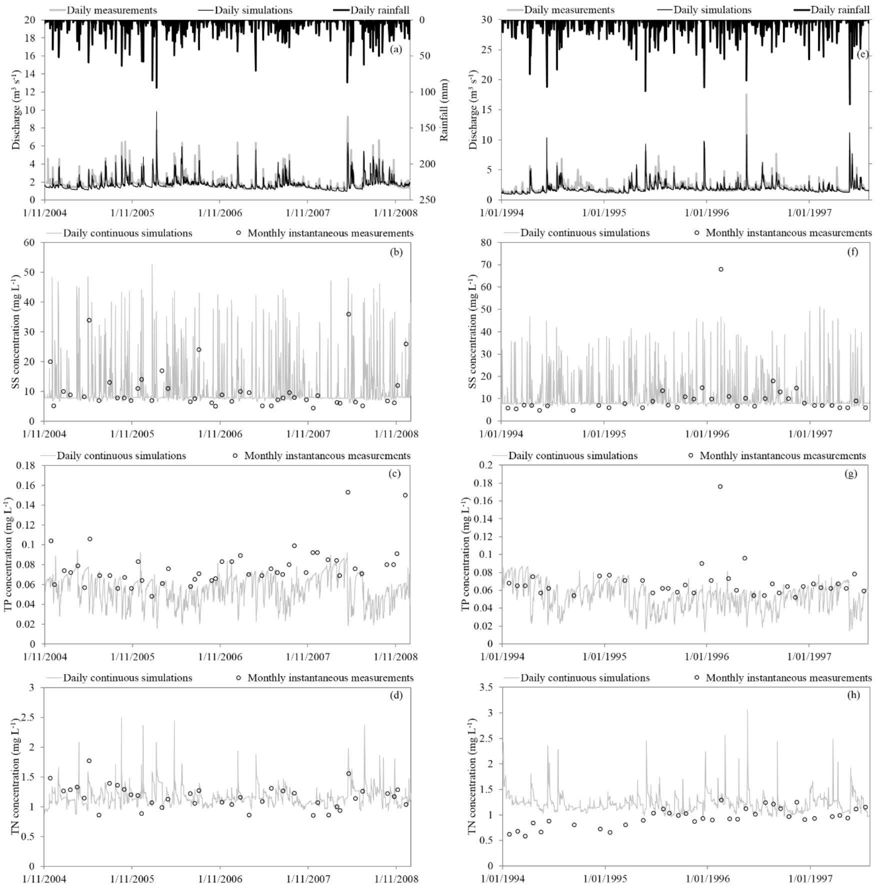

Figure 3. Measurements and daily mean simulated values of discharge, suspended sediment (SS), total phosphorus (TP) and total nitrogen (TN) during calibration **(a–d)** and validation **(e–h)**. Measured daily mean discharge was calculated from 15 min observations and measured concentrations of SS, TP and TN correspond to monthly grab samples.

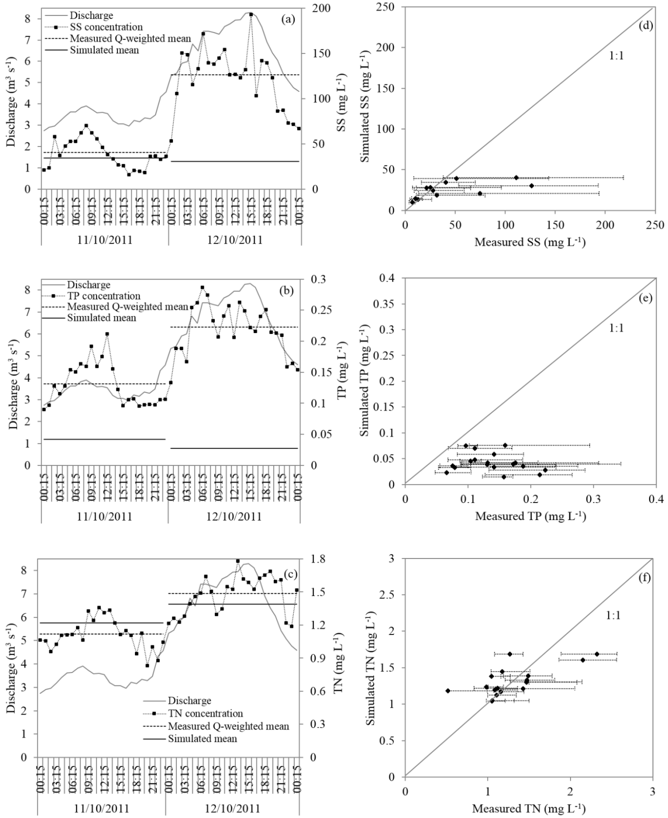

Figure 4. Example of hourly measurements, calculated discharge (Q)-weighted mean concentrations and simulated daily mean concentrations of suspended sediment (SS), total phosphorus (TP) and total nitrogen (TN) for two days during one storm event **(a–c)**. Comparison includes Q-weighted mean concentrations for 24 h periods (horizontal bars show range of hourly measurements) during storm events (2010–2012) and simulated daily mean estimates of SS, TP and TN **(d–f)**.

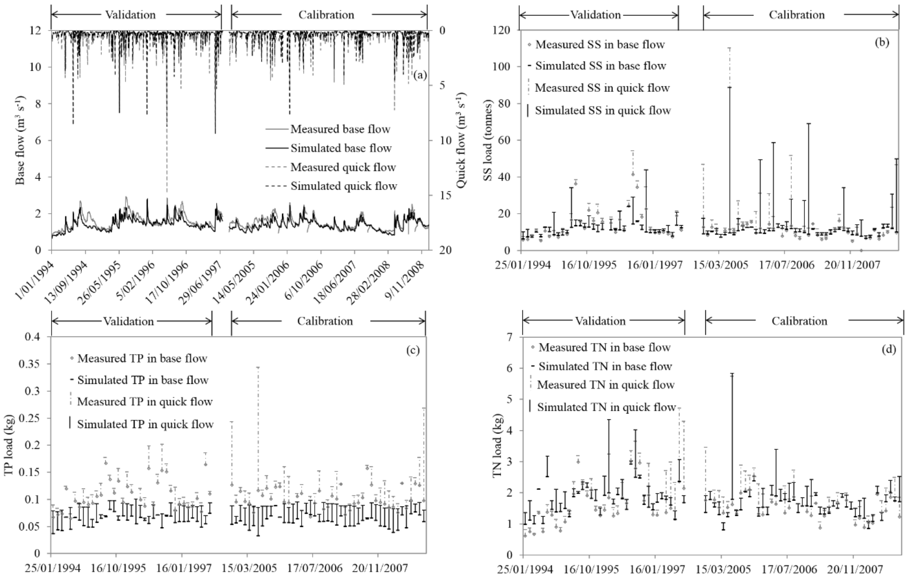

Figure 5. Measurements and simulations derived using the calibrated set of parameter values. Data are shown separately for base flow and quick flow. **(a)** Daily mean base flow and quick flow; **(b)** suspended sediment (SS) load; **(c)** total phosphorus (TP) load; **(d)** total nitrogen (TN) load. Vertical lines in **(b–d)** show the contaminant load in quick flow. Time series relate to calibration (2004–2008) and validation (1994–1997) periods (note time discontinuity). Measured instantaneous loads of SS, TP, and TN correspond to monthly grab samples.

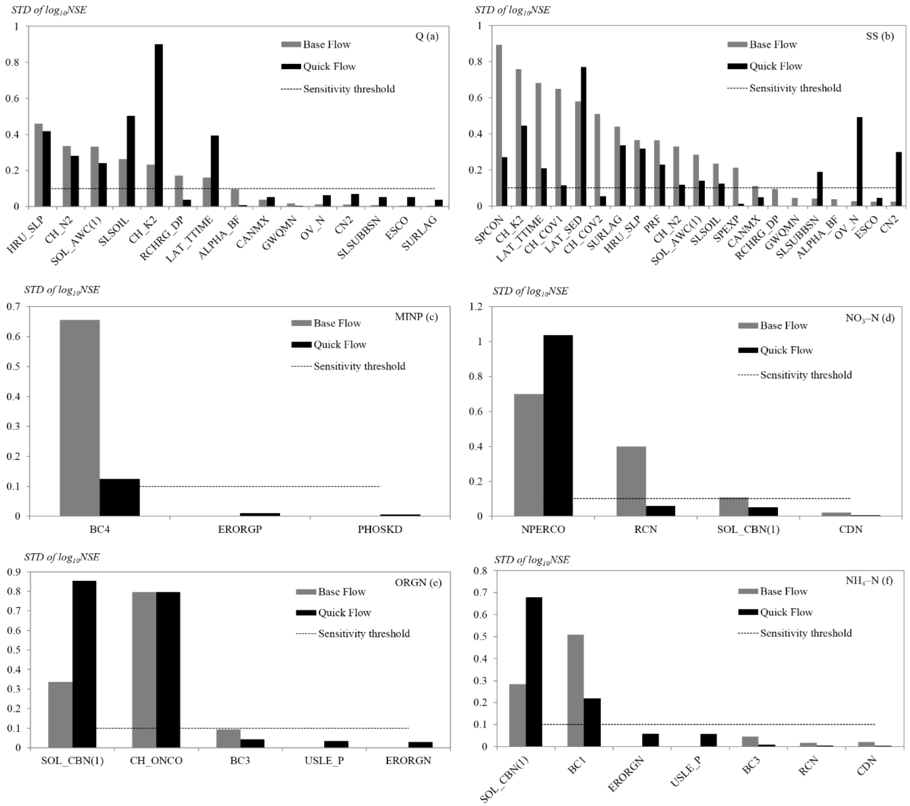

Figure 6. Parameter sensitivity for base flow and quick flow based on one-at a-time (OAT) sensitivity analysis for each simulated variable: **(a)** *Q* (discharge); **(b)** SS (suspended sediment); **(c)** MINP (mineral phosphorus); **(d)** NO_3–N (nitrate–nitrogen); **(e)** ORGN (organic nitrogen); **(f)** NH_4–N (ammonium–nitrogen). Parameter sensitivity is quantified as the variation in standard deviation of $\log_{10}$-transformed Nash–Sutcliffe efficiency (NSE) with a sensitivity threshold assigned as 0.1 (see Sect. 2.5). Definitions of each parameter are shown in Table 3.

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