

Effects of hydrologic conditions on SWAT model performance and parameter sensitivity for a small, mixed land use catchment in New Zealand

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Abstract

The Soil Water Assessment Tool (SWAT) was configured for the Puarenga Stream catchment (77 km²), 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. Model validation was performed using two datasets: 1) monthly instantaneous measurements of suspended sediment (SS), total phosphorus (TP) and total nitrogen (TN) concentrations; and 2) high-frequency (1–2 h) data measured during rainfall events. Monthly instantaneous TP and TN concentrations were generally not reproduced well (24% bias for TP, 27% bias for TN, and $R^2 < 0.1$, $NSE < 0$ for both TP and TN), in contrast to SS concentrations ($< 1\%$ bias; R^2 and NSE both > 0.75) during model validation. Comparison of simulated daily mean SS, TP and TN concentrations with daily mean discharge-weighted high-frequency measurements during storm events indicated that model predictions during the high rainfall period considerably underestimated concentrations of SS (44% bias) and TP (70% bias), while TN concentrations were comparable ($< 1\%$ bias; R^2 and NSE both ~ 0.5). This comparison highlighted the potential for model error associated with quick-

1 flow fluxes in flashy lower-order streams to be underestimated compared with
2 low-frequency (e.g. monthly) measurements derived predominantly from base
3 flow measurements. To address this, we recommend that high-frequency, event-
4 based monitoring data are used to support calibration and validation. Simulated
5 discharge, SS, TP and TN loads were partitioned into two components (base flow
6 and quick flow) based on hydrograph separation. A manual procedure (one-at-a-
7 time sensitivity analysis) was used to quantify parameter sensitivity for the two
8 hydrologically-separated regimes. Several SWAT parameters were found to have
9 different sensitivities between base flow and quick flow. Parameters relating to
10 main channel processes were more sensitive for the base flow estimates, while
11 those relating to overland processes were more sensitive for the quick flow
12 estimates. This study has important implications for identifying uncertainties in
13 parameter sensitivity and performance of hydrological models applied to
14 catchments with large fluctuations in stream flow, and in cases where models are
15 used to examine scenarios that involve substantial changes to the existing flow
16 regime.

17

18 **1 Introduction**

19 Catchment models are valuable tools for understanding natural processes
20 occurring at basin scales and for simulating the effects of different management
21 regimes on soil and water resources (e.g. Cao et al., 2006). Model applications
22 may have uncertainties as a result of errors associated with the forcing variables,
23 measurements used for calibration, and conceptualisation of the model itself
24 (Lindenschmidt et al., 2007). The ability of catchment models to simulate
25 hydrological processes and pollutant loads can be assessed through analysis of
26 uncertainty or errors during a calibration process that is specific to the application
27 domain (White and Chaubey, 2005).

28 The Soil and Water Assessment Tool (SWAT) model is increasingly used
29 to predict discharge, sediment and nutrient loads on a temporally resolved basis,
30 and to quantify material fluxes from a catchment to the downstream receiving
31 environment such as a lake (e.g. Nielsen et al., 2013). The SWAT model is
32 physically-based and provides distributed descriptions of hydrologic processes at
33 sub-basin scale (Arnold et al., 1998; Neitsch et al., 2011). It has numerous

1 parameters, some of which can be fixed on the basis of pre-existing catchment
2 data (e.g. soil maps) or knowledge gained in other studies. However, values for
3 other parameters need to be assigned during a calibration process as a result of
4 complex spatial and temporal variations that are not readily captured either
5 through measurements or within the model algorithms themselves (Boyle et al.,
6 2000). Such parameter values assigned during calibration are therefore lumped,
7 i.e., they integrate variations in space and/or time and thus provide an
8 approximation for real values which often vary widely within a study catchment.
9 Model calibration is an iterative process whereby parameters are adjusted to the
10 system of interest by refining model predictions to fit closely with observations
11 under a given set of conditions (Moriassi et al., 2007). Manual calibration depends
12 on the system used for model application, the experience of the modellers, and
13 knowledge of the model algorithms. It tends to be subjective and time-consuming.
14 By contrast, auto-calibration provides a less labour-intensive approach by using
15 optimisation algorithms (Eckhardt and Arnold, 2001). The Sequential Uncertainty
16 Fitting (SUFI-2) procedure has previously been applied to auto-calibrate
17 discharge parameters in a SWAT application for the Thur River, Switzerland
18 (Abbaspour et al., 2007), as well as for groundwater recharge, evapotranspiration
19 and soil storage water considerations in West Africa (Schuol et al., 2008). Model
20 validation is subsequently performed using measured data that are independent of
21 those used for calibration (Moriassi et al., 2007).

22 Values for hydrological parameter values in the SWAT model can vary
23 temporally. Cijin et al. (2010) found that the optimum calibrated values for
24 hydrological parameters varied with different flow regimes (low, medium and
25 high), thus suggesting that SWAT model performance can be optimised by
26 assigning parameter values based on hydrological characteristics. Other work has
27 similarly demonstrated benefits from assigning separate parameter values to low,
28 medium, and high discharge periods (Yilmaz et al., 2008), or based on whether a
29 catchment is in a dry, drying, wet or wetting state (Choi and Beven, 2007). Such
30 temporal dependence of model parameterisation on hydrologic conditions has
31 implications for model performance. Krause et al. (2005) compared different
32 statistical metrics of hydrological model performance separately for base-flow
33 periods and storm events to evaluate the performance. The authors found that the
34 logarithmic form of the Nash-Sutcliffe efficiency (NSE) value provided more

1 information on the sensitivity of model performance for discharge simulations
2 during storm events, while the relative form of NSE was better for base flow
3 periods. Similarly, Guse et al. (2014) investigated temporal dynamics of
4 sensitivity of hydrological parameters and SWAT model performance using
5 Fourier amplitude sensitivity test (Reusser et al., 2011) and cluster analysis
6 (Reusser et al., 2009). The authors found that three groundwater parameters were
7 highly sensitive during quick flow, while one evaporation parameter was most
8 sensitive during base flow, and model performance was also found to vary
9 significantly for the two flow regimes. Zhang et al. (2011) calibrated SWAT
10 hydrological parameters for periods separated on the basis of six climatic indexes.
11 Model performance improved when different values were assigned to parameters
12 based on six hydroclimatic periods. Similarly, Pfannerstill et al. (2014) found that
13 assessment of model performance was improved by considering an additional
14 performance statistic for very low-flow simulations amongst five hydrologically-
15 separated regimes.

16 To date, analysis of temporal dynamics of SWAT parameters has
17 predominantly focussed on simulations of discharge rather than water quality
18 constituents. This partly reflects the paucity of comprehensive water quality data
19 for many catchments; near-continuous discharge data can readily be collected but
20 this is not the case for water quality parameters such as suspended sediment or
21 nutrient concentrations. Data collected in monitoring programmes that involve
22 sampling at regular time intervals (e.g. monthly) are often used to calibrate water
23 quality models, but these are unlikely to fully represent the range of hydrologic
24 conditions in a catchment (Bieroza et al., 2014). In particular, water quality data
25 collected during storm-flow periods are rarely available for SWAT calibration,
26 thus prohibiting opportunities to investigate how parameter sensitivity varies
27 under conditions which can contribute disproportionately to nutrient or sediment
28 transport, particularly in lower-order catchments (Chiwa et al., 2010; Abell et al.,
29 2013). Failure to fully consider storm-flow processes could therefore result in
30 overestimation of model performance. Thus, further research is required to
31 examine how water quality parameters vary during different flow regimes and to
32 understand how model uncertainty may vary under future climatic conditions that
33 affect discharge regimes (Brigode et al., 2013).

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

13 **2 Methods**

14 **2.1 Study area**

15 The Puarenga Stream is the second-largest surface inflow to Lake Rotorua (Bay
16 of Plenty, New Zealand) and drains a catchment of 77 km². The catchment is
17 situated in the central North Island of New Zealand, which has a warm temperate
18 climate. Annual mean temperature at Rotorua Airport (Fig. 1a) is 15±4 °C and
19 annual mean evapotranspiration is 714 mm yr⁻¹ (1993–2012; National Climatic
20 Data Centre; available at <http://cliflo.niwa.co.nz/>). Annual mean precipitation at
21 Kaituna rain gauge (Fig. 1a) is 1500 mm yr⁻¹ (1993–2012; Bay of Plenty Regional
22 Council). The catchment is relatively steep (mean slope = 9%; Bay of Plenty
23 Regional Council) with predominantly pumice soils that have high macroporosity,
24 resulting in high infiltration rates and substantial sub-surface lateral flow
25 contributions to stream channels. Two cold-water springs (Waipa Spring and
26 Hemo Spring) and one geothermal spring (Fig. 1b) are located in the catchment
27 area. Two cold-water springs have annual mean discharge of ~0.19 m³ s⁻¹
28 (Rotorua District Council) and one geothermal spring has annual mean discharge
29 of ~0.12 m³ s⁻¹ (White et al., 2004).

30 The predominant land use (47%) is exotic forest (*Pinus radiata*).
31 Approximately 26% is managed pastoral farmland, 11% mixed scrub and 9%
32 indigenous forest. Since 1991, treated wastewater has been pumped from the
33 Rotorua Wastewater Treatment Plant and spray-irrigated over 16 blocks of total

1 area of 1.93 km² in the Whakarewarewa Forest (Fig. 1a). Following this, it took
2 approximately four years before elevated nitrate concentrations were measured in
3 the receiving waters of the Puarenga Stream (Lowe et al., 2007). Prior to 2002, the
4 irrigation schedule entailed applying wastewater to two blocks per day so that
5 each block was irrigated approximately weekly. Since 2002, 10 to 14 blocks have
6 been irrigated simultaneously at daily frequency. Over the entire period of
7 irrigation, nutrient concentrations in the irrigated water have gradually decreased
8 as improvements in treatment of the wastewater have been made (Lowe et al.,
9 2007).

10 Measurements from the Forest Research Institute (FRI) stream–gauge (1.7
11 km upstream of Lake Rotorua; Fig. 1b) were considered representative of the
12 downstream/outlet conditions of the Puarenga Stream. The FRI stream–gauge was
13 closed in mid 1997, then reopened late in 2004 (Environment Bay of Plenty,
14 2007). Annual mean discharge at this site is 2.0 m³ s⁻¹ (1994–1997 and 2004–
15 2008; Bay of Plenty Regional Council). The Puarenga Stream receives a high
16 proportion of flow from groundwater stores and has only moderate seasonality in
17 discharge. On average, the lowest mean daily discharge is during summer
18 (December to February; 1.7 m³ s⁻¹) and the highest mean daily discharge is during
19 winter (June to August; 2.4 m³ s⁻¹). Discharge records during 1998–2004 were
20 intermittent and this precluded a detailed comparison of measured and simulated
21 discharge during that period. In July 2010, the gauge was repositioned 720 m
22 downstream to the State Highway 30 (SH 30) bridge (Fig. 1b).

23 **2.2 Model configuration**

24 SWAT input data requirements included a digital elevation model (DEM),
25 meteorological records, records of springs and water abstraction, soil
26 characteristics, land use classification, and management schedules for key land
27 uses (pastoral farming, wastewater irrigation, and timber harvesting). The SWAT
28 model (version SWAT2009_rev488) was run on an hourly time step, but daily
29 mean simulation outputs were used for this study.

30 The DEM was used to delineate boundaries of the whole catchment and
31 individual sub–catchments, with a stream map used to ‘burn-in’ channel locations
32 to create accurate flow routings. Hourly rainfall estimates were used as hydrologic
33 forcing data. The Penman–Monteith method (Monteith, 1965) was used to

1 calculate evapotranspiration (ET) and potential ET. The Green and Ampt (1911)
2 method was used to calculate infiltration, rather than the SCS curve number
3 method. Therefore, the hourly rainfall/Green & Ampt infiltration/hourly routing
4 method (Neitsch et al., 2011) was chosen to simulate upland and in-stream
5 processes. Ten sub-catchments were represented in the Puarenga Stream
6 catchment, each comprising numerous Hydrologic Response Units (HRUs). Each
7 HRU aggregates cells with the same combination of land cover, soil, and slope. A
8 total of 404 HRUs was defined in the model. Runoff and nutrient transport were
9 predicted separately within SWAT for each HRU, with predictions summed to
10 obtain the total for each sub-catchment.

11 Descriptions and sources of the data used to configure the SWAT model
12 are given in Table 1. There were a total of 197 model parameters. Values of
13 SWAT parameters were assigned based on: i) measured data (e.g. some of the soil
14 parameters; Table 1); ii) literature values from published studies of similar
15 catchments (e.g. parameters for dominant land uses; Table 2); or iii) by calibration
16 where parameters were not otherwise prescribed.

17 SWAT simulates loads of ‘mineral phosphorus’ (MINP) and ‘organic
18 phosphorus’ (ORGP) of which the sum is total phosphorus (TP). The MINP
19 fraction represents soluble P either in mineral or in organic form, while ORGP
20 refers to particulate P bound either by algae or by sediment (White et al., 2014).
21 Soluble P may be taken up during algae growth, or released from benthic
22 sediment. This fraction can be transformed to particulate P contained in algae or
23 sediment.

24 SWAT simulates loads of nitrate–nitrogen ($\text{NO}_3\text{-N}$), ammonium–nitrogen
25 ($\text{NH}_4\text{-N}$) and organic nitrogen (ORGN), the sum of which is total nitrogen (TN).
26 Nitrogen parameters were auto-calibrated for each N fraction. The SWAT model
27 does not account for the initial nitrate concentration in shallow aquifers, as also
28 noted by Conan et al. (2003). Ekanayake and Davie (2005) indicated that SWAT
29 underestimated N loading from groundwater and suggested a modification by
30 adding a background concentration of nitrate in streamflow to represent
31 groundwater nitrate contributions. Over the period of the first five years of
32 wastewater irrigation, nitrate concentrations in shallow groundwater draining the
33 Waipa Stream sub-catchment were estimated to have increased by c. 0.44 mg L^{-1}
34 (Paku, 2001). SWAT has no capability to dynamically adjust the groundwater

1 concentration during a simulation run. Therefore we added 0.44 mg N L⁻¹ to all
2 model simulations of TN concentration assuming that groundwater concentrations
3 had equilibrated with the applied wastewater nitrogen.

4 **2.3 Model calibration and validation**

5 Daily mean discharge was firstly calibrated based on daily mean values of 15–
6 minute measurements (Table 3). Water quality variables were then calibrated in
7 the sequence: SS, TP and TN. Modelled mean daily concentrations were
8 compared with concentrations measured during monthly grab sampling, with
9 monthly measurements assumed equal to daily mean concentrations (Table 3).
10 One year (1993) was used for model warmup. The calibration period was from
11 2004 to 2008 and the validation period was from 1994 to 1997. A validation
12 period that pre-dated the calibration period was chosen because discharge records
13 were available for two separate periods (1994–1997 and post 2004). In addition,
14 the operational regime for the wastewater irrigation has varied since operations
15 began in 1991, with a marked change occurring in 2002 when operations switched
16 from applying the wastewater load to two blocks (rotated daily for a total of 14
17 blocks in a week; i.e., each block irrigated weekly), to 10–14 blocks each irrigated
18 daily. This operational regime continues today and we therefore decided to assign
19 the most recent (post 2002) period (2004–2008) to calibration to ensure that the
20 model was configured to reflect current operations.

21 Parameter values that were not derived from measurements or the
22 literature were assigned based on either automated or manual calibration (Table 4).
23 Manual calibration was undertaken for 11 parameters related to TP, while a
24 Sequential Uncertainty Fitting (SUFI-2) procedure was applied to auto-calibrate
25 21 parameters for discharge simulations, nine parameters for SS simulations, and
26 17 parameters related to TN. The SUFI-2 procedure has been integrated into the
27 SWAT Calibration and Uncertainty Program (SWAT-CUP). SUFI-2 is a
28 procedure that efficiently quantifies and constrains parameter uncertainties/ranges
29 from default ranges with the fewest number of iterations (Abbaspour et al., 2004),
30 and has been shown to provide optimal results relative to the use of alternative
31 algorithms (Wu and Chen, 2015). SUFI-2 involves Latin hypercube sampling
32 (LHS), which is a method that generates a sample of plausible parameter values
33 from a multidimensional distribution and ensures that samples cover the entire

1 parameter space, therefore ensuring that the optimum solution is not a local
2 minimum (Marino et al., 2008).

3 The SUFI-2 procedure analyses relative sensitivities of parameters by
4 randomly generating combinations of values for model parameters (Abbaspour et
5 al., 2014). A sample size of 1000 was chosen for each iteration of LHS, resulting
6 in 1000 combinations of parameters and 1000 simulations. Model performance
7 was quantified for each simulation based on the Nash–Sutcliffe efficiency (*NSE*).
8 An objective function was defined as a linear regression of a combination of
9 parameter values generated by each LHS against the *NSE* value calculated from
10 each simulation. Each compartment was not given weight to formulate the
11 objective function because only one variable was specifically focused on at each
12 time. A parameter sensitivity matrix was then computed based on the changes in
13 the objective function after 1000 simulations. Parameter sensitivity was quantified
14 based on the *p* value from a Student’s t-test, which was used to compare the mean
15 of simulated values with the mean value of measurements (Rice, 2006). A
16 parameter was deemed sensitive if $p \leq 0.05$ after 1000 simulations (one iteration).
17 Numerous iterations of LHS were conducted. Values of *p* from numerous
18 iterations were averaged for each parameter, and the frequency of iterations where
19 a parameter was deemed sensitive was summed. Rankings of relative sensitivities
20 of parameters were developed based on how frequently the sensitive parameter
21 was identified and the averaged value of *p* calculated from several iterations. The
22 most sensitive parameter was determined based on the frequency that the
23 parameter was deemed sensitive, and the smallest average *p*-value from all
24 iterations.

25 SUFI-2 considers two criteria to constrain uncertainty in each iteration.
26 One is the P-factor, the percentage of measured data bracketed by 95% prediction
27 uncertainty (95PPU). Another is the R-factor, the average thickness of the 95PPU
28 band divided by the standard deviation of measured data. A range was first
29 defined for each parameter based on a synthesis of ranges from similar studies or
30 from the SWAT default range. Parameter ranges were updated after each iteration
31 based on the computation of upper and lower 95% confidence limits. The 95%
32 confidence interval and the standard deviation of a parameter value were derived
33 from the diagonal elements of the covariance matrix, which was calculated from

1 the sensitivity matrix and the variance of the objective function. Steps and
2 equations used in the SUFI-2 procedure to constrain parameter ranges are
3 outlined by Abbaspour et al. (2004).

4 The total numbers of iterations performed for each simulated variable (Q,
5 SS, MINP, ORGN, NH₄-N and NO₃-N) reflected the numbers required to ensure
6 that > 90% of measured data were bracketed by simulated output and the R-factor
7 was close to one. The ‘optimal’ parameter value was obtained when the Nash–
8 Sutcliffe efficiency (NSE) criterion was satisfied (NSE > 0.5; Moriasi et al., 2007).
9 Auto-calibrated parameters for simulations of Q, SS, and TN were changed by
10 absolute values within the given ranges. Some of those given ranges were
11 restricted based on the optimum values calibrated in similar studies. Parameter
12 values for TP simulations were manually-calibrated based on the relative percent
13 deviation from the predetermined values of those auto-calibrated parameters for
14 MINP simulations, given by the objective functions (e.g., NSE). Parameters
15 related to the physical characteristics of the catchment were not changed because
16 their values were considered to be representative of the catchment characteristics.

17 In addition, high-frequency (1–2 h) water quality sampling was
18 undertaken at the FRI stream-gauge during 2010–2012 (Table 3) to derive
19 estimates of daily mean contaminant loads during storm events. Samples were
20 analysed for SS (nine events), TP and TN (both 14 events) over sampling periods
21 of 24–73 h. The sampling programme was designed to encompass pre-event base
22 flow, storm generated quick flow and post-event base flow (Abell et al., 2013).
23 These data permitted calculation of daily discharge-weighted (Q-weighted) mean
24 concentrations to compare with modelled daily mean estimates. We did not use
25 the high-frequency observations to calibrate the model, because of the limited
26 number of high-frequency (1–2 h) samples (nine events for SS and 14 events for
27 TP and TN in 2010–2012). The use of the high-frequency observations for model
28 validation allowed to examine how the model performed during short (1–3 day)
29 high flow periods. The Q-weighted mean concentrations C_{QWM} were calculated as:

30
$$C_{QWM} = \frac{\sum_{i=1}^n C_i Q_i}{\sum_{i=1}^n Q_i} \quad (1)$$

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

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 was 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:

$$C_{sep} = \frac{Q_q \times C'_q + Q_b \times C'_b}{Q_q + Q_b} \quad (2)$$

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).

To ensure that C'_q is positive, C'_b is constrained to be the minimum of $\overline{C_{sep}}$ and C_{sep} . Measured and simulated base flow and quick flow contaminant loads were then calculated.

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), based on the ranking of relative sensitivities of parameters that were identified by randomly generating combinations of values for model parameters for each individual variable using the SUFI-2 procedure. OAT sensitivity analysis was then employed by varying the parameter of interest among ten equidistant values within the default range. The natural logarithm was used by Krause et al. (2005) and therefore the standard deviation (STD) of the ln-transformed NSE was used to indicate parameter sensitivity for the two flow regimes.

Parameters were ranked from most to least sensitive on the basis of the sensitivity metric (STD of ln-transformed NSE), using a value of 0.2 as a threshold above which parameters were deemed particularly 'sensitive'. The

threshold value of 0.2 was chosen in this study, based on the median value derived from the calculations of the *STD* of \ln -transformed NSE. Methods used to separate the two flow constituents and to quantify parameter sensitivity are illustrated in Fig. 2.

2.5 Model evaluation

Model goodness-of-fit was assessed graphically and quantified using coefficient of determination (R^2), Nash–Sutcliffe efficiency (NSE) and percent bias (PBIAS; Table 5). R^2 (range 0 to 1) and NSE (range $-\infty$ to 1) values are commonly used to evaluate SWAT model performance (Gassman et al., 2007). PBIAS value indicates the average tendency of simulated outputs to be larger or smaller than observations (Gupta et al., 1999).

Model uncertainty was evaluated by two criteria: R-factor and P-factor (see Section 2.3). They were used to constrain parameter ranges during the calibration using measured Q and loads of SS, MINP, ORGN, $\text{NH}_4\text{-N}$ and $\text{NO}_3\text{-N}$ in the SUFI-2 procedure. The R software (R Development Core Team) was used to graphically show the 95% confidence and prediction intervals for measurement data (Neyman, 1937) and model prediction intervals (Seymour, 1993) for Q and concentrations of SS, TP and TN during the calibration period (2004–2008).

3 Results

3.1 Model performance and uncertainty

Numerous rounds (each comprising 1000 iterations) of LHS were conducted for each simulated variable until the performance criteria were satisfied. The total number of rounds of LHS for each simulated variable was as follows (number in parentheses): Q (7), SS (7), MINP (11), ORGN (10), $\text{NH}_4\text{-N}$ (4) and $\text{NO}_3\text{-N}$ (4). The parameters that provided the best statistical outcomes (i.e, best match to observed data) are given in Table 4. Two criteria (R-factor and P-factor) were used to show model uncertainties for simulations of discharge and contaminant loads, with values as follows: Q (0.97, 0.43), SS (0.48, 0.19), MINP (2.64, 0.14), ORGN (0.47, 0.17), $\text{NH}_4\text{-N}$ (1.16, 0.56) and $\text{NO}_3\text{-N}$ (1.2, 0.29). Model uncertainties for simulations of Q and SS, TP and TN concentrations are shown in Fig. 6.

1 Modelled and measured base flow showed high correspondence, although
2 measured daily mean discharge during storm peaks was often underestimated (Fig.
3 3a and 3e). Annual mean percentages of lateral flow recharge, shallow aquifer
4 recharge and deep aquifer recharge to total water yield were predicted by SWAT
5 as 30%, 10%, 58%, respectively. Modelled SS concentrations overestimated
6 measurements of monthly grab samples by an average of 18.3% during calibration
7 and 0.32% during validation (Fig. 3b and 3f). Measured TP concentrations in
8 monthly grab samples were underestimated by 23.8% during calibration (Fig. 3c)
9 and 24.5% during validation (Fig. 3g). Similarly, measured TP loads were
10 underestimated by 34.5% and 38.4%, during calibration and validation,
11 respectively. Modelled and measured TN concentrations were generally better
12 aligned during base flow (Fig. 3d), apart from a mismatch prior to 1996 when
13 monthly measured TN concentrations were substantially lower than model
14 predictions, although the concentrations gradually increased (Fig. 3h) during the
15 validation period (1994–1997). The average measured TN load increased from
16 134 kg N d⁻¹ prior to 1996, to 190 kg N d⁻¹ post 1996. The comparable increase in
17 modelled TN load was 167 kg N d⁻¹ to 205 kg N d⁻¹, respectively.

18 Statistical evaluations of goodness-of-fit are shown in Table 6. The R²
19 values for discharge were 0.77 for calibration and 0.68 for validation,
20 corresponding to model performance ratings (cf. Moriasi et al., 2007) of ‘very
21 good’ and ‘good’ (Table 5). Similarly, the NSE values for discharge were 0.73
22 (good) for calibration and 0.62 (satisfactory) for validation. Positive PBIAS (7.8%
23 for calibration and 8.8% for validation) indicated a tendency for underestimation
24 of daily mean discharge, however, the low magnitude of PBIAS values
25 corresponded to a performance rating of ‘very good’. The R² values for SS were
26 0.42 (unsatisfactory) for calibration and 0.80 for validation (very good). Similarly,
27 the NSE values for SS were -0.08 (unsatisfactory) for calibration and 0.76 (very
28 good) for validation. The model did not simulate trends well for monthly
29 measured TP and TN concentrations. The R² values for TP and TN were both <
30 0.1 (unsatisfactory) during calibration and validation and NSE values were both <
31 0 (unsatisfactory). Values of PBIAS corresponded to ‘good’ or ‘very good’
32 performance ratings for TP and TN.

1 Observed Q-weighted daily mean concentrations derived from hourly
2 measurements and simulated daily mean concentrations of SS, TP and TN during
3 an example two-day storm event are shown in Fig. 4a–4c. The simulations of SS
4 and TN concentrations were somewhat better than for TP. Comparisons of Q-
5 weighted daily mean concentrations (C_{QWM}) during storm events from 2010 to
6 2012 are shown in Fig. 4d–4f for SS (nine events), TP and TN (both 14 events).
7 The C_{QWM} of TP exceeded the simulated daily mean by between 0.02 and 0.2 mg
8 $P L^{-1}$, and on average, the model underestimated measurements by 69.4% (Fig. 4e).
9 Although R^2 and NSE values for C_{QWM} of TN were unsatisfactory (Table 6), they
10 were both close to the threshold for satisfactory performance (0.5). For C_{QWM} of
11 SS and TP, R^2 and NSE values indicated that the model performance was
12 unsatisfactory. The PBIAS value of -0.87 for C_{QWM} of TN corresponded to model
13 performance ratings of ‘very good’, while the PBIAS values for C_{QWM} of SS and
14 TP were 43.9 and 69.4, respectively, indicating satisfactory model performance.

15 Measured and simulated discharge and contaminant loads separated for the
16 two flow regimes (base flow and quick flow) are shown in Fig. 5. Model
17 performance statistics differed between the two flow regimes (Table 7).
18 Simulations of discharge and constituent loads under quick flow were more
19 closely related to the measurements (i.e., higher values of R^2 and NSE) than
20 simulations under base flow. Base flow TN load simulations during the validation
21 period showed better model performance than simulations under quick flow.
22 Additionally, measurements under quick flow were better reproduced by the
23 model than the measurements for the whole simulation period. Simulations of
24 contaminant loads matched measurements much better than for contaminant
25 concentrations, as indicated by statistical values for model performance given in
26 Table 6 and 7.

27 **3.2 Separated parameter sensitivity**

28 Based on the ranking of relative sensitivities of hydrological and water quality
29 parameters derived from the SUFI-2 procedure (see Table 8), the OAT sensitivity
30 analysis undertaken separately for base flow and quick flow identified three
31 parameters that most influenced the quick flow estimates, and five parameters that
32 most influenced the base flow estimates (parameters above the dashed line in Fig.
33 7a). Channel hydraulic conductivity (CH_K2) is used to estimate the peak runoff

1 rate (Lane, 1983). Lateral flow slope length (SLSOIL) and lateral flow travel time
2 (LAT_TIME) have an important controlling effect on the amount of lateral flow
3 entering the stream reach during quick flow. Both slope (HRU_SLP) and soil
4 available water content (SOL_AWC) were particularly sensitive for the base flow
5 simulation because they affect lateral flow within the kinematic storage model in
6 SWAT (Sloan and Moore, 1984). The aquifer percolation coefficient
7 (RCHRG_DP) and the base flow alpha factor (ALPHA_BF) strongly influenced
8 base flow calculations (Sangrey et al., 1984), as did the channel Manning's N
9 value (CH_N2) which is used to estimate channel flow (Chow, 2008).

10 For SS loads, 12 and four parameters, respectively, were identified as
11 sensitive in relation to the simulations of base flow and quick flow (parameters
12 above the dashed line in Fig. 7b). Parameters that control main channel processes
13 (e.g. CH_K2 and CH_N2) and subsurface water transport processes (e.g.
14 LAT_TIME and SLSOIL) were found to be much more sensitive for base flow SS
15 load estimations. Exclusive parameters for SS estimations, such as SPCON (linear
16 parameter), PRF (peak rate adjustment factor), SPEXP (exponent parameter),
17 CH_COV1 (channel erodibility factor), and CH_COV2 (channel cover factor)
18 were found to be much more sensitive in base flow SS load, while LAT_SED (SS
19 concentration in lateral flow and groundwater flow) was more sensitive in quick
20 flow SS load. Parameters that control overland processes, e.g. CN2 (the curve
21 number), OV_N (overland flow Manning's N value) and SLSUBBSN (sub-basin
22 slope length), were found to be much more sensitive for quick flow SS load
23 estimations.

24 Of the sensitive parameters, BC4 (ORGP mineralization rate) was
25 particularly sensitive for the simulation of base flow MINP load (Fig. 7c). RCN
26 (nitrogen concentration in rainfall) related specifically to the dynamics of the base
27 flow NO₃-N load and NPERCO (nitrogen percolation coefficient) significantly
28 affected quick flow NO₃-N load (Fig. 7d). Parameter CH_ONCO (channel ORGN
29 concentration) similarly affected both flow components of ORGN load (Fig. 7e)
30 and SOL_CBN (organic carbon content) was most sensitive for the simulations of
31 quick flow ORGN and NH₄-N loads. Parameter BC1 (nitrification rate in reach)
32 was particularly sensitive for the simulation of base flow NH₄-N load (Fig. 7f).

33

4 Discussion

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 the 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.

4.1 Temporal dynamics of model performance

The modelled estimates of deep aquifer recharge (58%) and combined lateral flow and shallow aquifer recharge (40%) were comparable with estimates derived by Rutherford et al. (2011), who used an alternative catchment model to derive respective estimates of 30% and 70% for these two fluxes. Our decision to deliberately select a validation period (1994–1997) during which the boundary conditions of the system (specifically anthropogenic nutrient loading) differed considerably from the calibration period allowed us to rigorously assess the capability of SWAT to accurately predict water quality under an altered management scenario (i.e. the purpose of most SWAT applications).

Overestimation of TN concentrations prior to 1996 reflects higher NO₃-N concentrations in groundwater during the calibration period (2004–2008) due to the wastewater irrigation operation. Nitrate concentrations appeared to reach a new quasi-steady state as wastewater loads and in-stream attenuation came into

1 balance. SWAT may not adequately represent the dynamics of groundwater
2 nutrient concentrations (Bain et al., 2012) particularly in the presence of changes
3 in catchment inputs (e.g., with start-up of wastewater irrigation). The
4 groundwater delay parameter was set to five years (cf. Rotorua District Council,
5 2006), but this did not appear to capture adequately the lag in response to
6 increases in stream nitrate concentrations following wastewater irrigation from
7 1991.

8 The poor fit between simulated daily mean TP concentrations and monthly
9 instantaneous measurements may partly reflect a mismatch between the dominant
10 processes affecting phosphorus cycling in the stream and those represented in
11 SWAT. The ORGP fraction that is simulated in SWAT includes both organic and
12 inorganic forms of particulate phosphorus, however, the representation of
13 particulate phosphorus cycling only focusses on organic phosphorus cycling, with
14 limited consideration of interactions between inorganic streambed sediments and
15 dissolved reactive phosphorus in the overlying water (White et al., 2014). This
16 contrasts with phosphorus cycling in the study stream where it has been shown
17 that dynamic sorption processes between the dissolved and particulate inorganic
18 phosphorus pools exert major control on phosphorus cycling (Abell and Hamilton,
19 2013).

20 Our finding that measured Q-weighted mean concentrations (C_{QWM}) of TP
21 and SS during storm events (2010–2012) were greatly underestimated relative to
22 simulated daily mean TP and SS concentrations has important implications for
23 studies that examine effects of altered flow regimes on contaminant transport. For
24 example, studies which simulate scenarios comprising more frequent large rainfall
25 events (associated with climate change predictions for many regions; IPCC, 2013)
26 may considerably underestimate projected future loads of SS and associated
27 particulate nutrients if only base flow water quality measurements (i.e. those
28 predominantly collected during ‘state of environment’ monitoring) are used for
29 calibration/validation (see Radcliffe et al., 2009 for a discussion of this issue in
30 relation to phosphorus). This is also reflected by the two model performance
31 statistics relating to validation of modelled SS concentrations using monthly grab
32 samples (predominantly base flow; ‘very good’) and C_{QWM} estimated during
33 storm sampling (‘unsatisfactory’) based on R^2 and NSE values.

4.2 Key uncertainties

Model uncertainty in this study may arise from four main factors: 1) model parameters; 2) forcing data; 3) in measurements used for evaluation of model fit, and; 4) model structure or algorithms (Lindenschmidt et al., 2007). The values of most parameters assigned for model calibration, although specific to different soil types (e.g. soil parameters), were lumped across land uses and slopes in this study. They integrated spatial and temporal variations, thus neglecting any variability throughout the study catchment. In terms of forcing data, the assumption of constant values of spring discharge rate and nutrient concentrations may inadequately reflect the temporal variability and therefore increase model uncertainty, although this should contribute little to the model error term. Most water quality data used for model calibration comprised monthly instantaneous samples taken during base flow conditions. The use of those measurements for model calibration would likely lead to considerable underestimation of constituent concentrations (notably SS and TP) due to failure to account for short-term high flow events. Inadequate representation of groundwater processes in the model structure is another key factor that is likely to affect model uncertainty, particularly for nitrogen simulations. The analysis of model performance based on datasets separated into base flow and quick flow constituents enabled uncertainties in the structure of hydrological models to be identified, denoted by different model performance between these two flow constituents. 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 (e.g., compare model performance statistics for prediction of nutrient concentrations in Table 6 with statistics for prediction of loads in Table 7). 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.

4.3 Temporal dynamics of parameter sensitivity

To date, studies of temporal variability of parameters have focused on hydrological parameters, rather than on water quality parameters. The characteristics of concentration–discharge relationships for SS and TP are different to that for TN (Abell et al., 2013). In quick flow, there is a positive relationship between Q and concentrations of SS and TP, reflecting mobilisation of sediments and associated particulate P. Total nitrogen concentrations declined slightly in quick flow, reflecting the dilution of nitrate from groundwater. 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 km²), 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.

1 (2010; relatively sensitive) likely reflects differences in catchment size. The
2 Puarenga Stream catchment (77 km²) is much smaller than the study catchment
3 (St Joseph River; 2800 km²) of Cibin et al. (2010) and, consequently, distances to
4 the main channel are much shorter, with less potential for attenuation of surface
5 runoff in off-channel storage sites. The curve number (CN2) parameter was found
6 to be insensitive in both this study and Shen et al. (2012), because surface runoff
7 was simulated based on the Green and Ampt method (1911) requiring the hourly
8 rainfall inputs, rather than the curve number equation which is an empirical model.
9 By contrast, the most sensitive parameters in our study are those that determine
10 the extent of lateral flow, an important contributor to streamflow in the catchment,
11 due to a general lack of ground cover under plantation trees and formation of
12 gully networks on steep terrain.

13 Parameters that control surface water transport processes (e.g. LAT_TIME
14 and SLSOIL) were found to be much more sensitive for base flow SS load
15 estimation than parameters that control groundwater processes (e.g. ALPHA_BF
16 and RCHRG_DP), reflecting the importance of surface flow processes for
17 sediment transport. Sensitive parameters for quick flow SS load estimation related
18 to overland flow processes (e.g. OV_N and SLSUBBSN), thus reflecting the fact
19 that sediment transport is largely dependent on rainfall-driven processes, as is
20 typical of steep and lower-order catchments. Modelled base flow NO₃-N loads
21 were most sensitive to the nitrogen concentration in rainfall (RCN) because of
22 rainfall as a predominant contributor to recharging base flow. The nitrogen
23 percolation coefficient (NPERCO) was more influential for quick flow NO₃-N
24 load estimation, probably indicating that the quick flow NO₃-N load is more
25 influenced by the mobilisation of concentrated nitrogen sources associated with
26 agriculture or treated wastewater distribution. High sensitivity of the organic
27 carbon content (SOL_CBN) for quick flow ORGN load estimates likely reflects
28 mobilisation of N associated with organic material following rainfall. The finding
29 that base flow NH₄-N load was more sensitive to nitrification rate in reach (BC1)
30 likely reflects that base flow provides more favourable conditions to complete this
31 oxidation reaction, as NH₄-N is less readily leached and transported. Similarly,
32 the ORGP mineralization rate (BC4) strongly influenced base flow MINP load
33 estimation, reflecting that base flow phosphorus transport is relatively more
34 influenced by cycling from channel bed stores, whereas quick flow phosphorus

1 transport predominantly reflects the transport of phosphorus that originated from
2 sources distant from the channel.

3

4 **5 Conclusions**

5 The performance of a SWAT model was quantified for different hydrologic
6 conditions in a small catchment with mixed land use. Discharge-weighted mean
7 concentrations of TP and SS measured during storm events were greatly
8 underestimated by SWAT, highlighting the potential for uncertainty to be greatly
9 underestimated in catchment model applications that are validated using a sample
10 of contaminant load measurements that is over-represented by measurements
11 made during base flow conditions. Monitoring programmes which collect high-
12 frequency and event-based data should be considered further to support more
13 robust calibration and validation of SWAT model applications. Accurate
14 simulation of nitrogen concentrations was constrained by the non-steady state of
15 groundwater nitrogen concentrations due to historic variability in anthropogenic
16 nitrogen applications to land. Improved representation of groundwater processes
17 in the model structure would reduce this aspect of model uncertainty. The
18 sensitivity of many parameters varied depending on the relative dominance of
19 base flow and quick flow, while curve number, soil evaporation compensation
20 factor, surface runoff lag coefficient, and groundwater delay were largely
21 invariant to the two flow regimes. Parameters relating to main channel processes
22 were more sensitive when estimating variables (particularly Q and SS) during
23 base flow, while those relating to overland processes were more sensitive for
24 simulating variables associated with quick flow. Temporal dynamics of both
25 parameter sensitivity and model performance due to dependence on hydrologic
26 conditions should be considered in further model applications. This study has
27 important implications for modelling studies of similar catchments that exhibit
28 short-term temporal fluctuations in stream flow. In particular these include small
29 catchments with relatively steep terrain and lower order streams with moderate to
30 high rainfall.

31

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24 2010.

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

Data	Application	Data description and configuration details	Source
Digital elevation model (DEM) & 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)
Spring discharge and nutrient loads	Point source (Fig. 1b)	Constant daily discharge and nutrient concentrations assigned to two cold-water springs (Waipa Spring and Hemo Spring) and one geothermal spring.	White et al., 2004; Proffit, 2009 (Unpublished Site Visit Report); Paku, 2001; Mahon, 1985; Glover, 1993; Rotorua District Council (pers. comm.)
Water abstraction volumes	Water use	Monthly water abstraction assigned to two cold-water springs.	Kusabs and Shaw, 2008; Jowett, 2008
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	22 soil types. Properties were quantified based on measurements (if available) or estimated using regression analysis to estimate properties for unmeasured functional horizons.	New Zealand Land Resource Inventory & digital soil map (available at http://smap.landcareresearch.co.nz)
Meteorological data	Meteorological forcing	Daily maximum and minimum temperature, daily mean relative humidity, daily global solar radiation, daily (9 am) surface wind speed and hourly precipitation.	Rotorua Airport Automatic Weather Station, National Climate Database (available at http://cliflo.niwa.co.nz/); Kaituna rain gauge (Fig. 1a)
Agricultural management practices	Agricultural management schedules	Stock density Applications of urea and di-ammonium phosphate Applications of manure-associated nutrients	Statistics New Zealand, 2006; Ledgard and Thorrold, 1998 Statistics New Zealand, 2006; Fert Research, 2009 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 (pers. comm.)

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

Land-cover type	Parameter	Definition	Value	Source
PINE (<i>Pinus radiata</i>)	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)
FRSE (Evergreen forest)	BN3	Proportion of N in biomass at maturity	0.00139	(Hopmans and Elms 2009)
	HVSTI	Percentage of biomass harvested	0	–
	BMX_TREES (tonnes ha ⁻¹)	Maximum biomass for a forest	372	(Hall et al., 2001)
PAST (Pastoral farm)	MAT_YRS (years)	Number of years for tree to reach full development	100	–
	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)

- 1 Table 3. Description of data used to calibrate the SWAT model. Data were measured at the Forest Research Institute (FRI) stream–
- 2 gauge and were considered representative of the downstream/outlet conditions of the Puarenga Stream.

Data	Application	Measurement data details	Source
Stream discharge measurements	Calibration (2004–2008) Validation (1994–1997)	15–min stream discharge data were measured at FRI stream–gauge (Fig. 1b) within the catchment and aggregated as daily mean values (1994–1997; 2004–2008).	BoPRC; Abell et al., 2013
Stream water quality measurements	Calibration (2004–2008) Validation ¹ (1994–1997; 2010–2012)	Monthly grab samples for determination of suspended sediment (SS), total phosphorus (TP) and total nitrogen (TN) concentrations (1994–1997; 2004–2008), and high–frequency event–based samples for concentrations of SS (nine events), TP and TN (both 14 events) at 1–2 h frequency (2010–2012), were also measured at FRI stream–gauge (Fig. 1b) within the catchment.	BoPRC; Abell et al., 2013

¹ Model validation was undertaken using two different datasets. The monthly measurements (1994–1997) were predominantly collected when base flow was the dominant contributor to stream discharge. Data from high–frequency sampling during rain events (2010–2012) were also used to validate model performance during periods when quick flow was high.

- 1 Table 4. Summary of calibrated SWAT parameters. Discharge (Q), suspended sediment (SS) and total nitrogen (TN) parameter
- 2 values were assigned using auto-calibration, while total phosphorus (TP) parameters were manually calibrated. SWAT default ranges
- 3 and input file extensions are shown for each parameter.

Parameter	Definition	Unit	Default range	Calibrated value
Q				
EVRCH.bsn	Reach evaporation adjustment factor		0.5–1	0.9
SURLAG.bsn	Surface runoff lag coefficient		0.05–24	15
ALPHA_BF.gw	Base flow alpha factor (0–1)		0.0071–0.0161	0.01
GW_DELAY.gw	Groundwater delay	d	0–500	500
GW_REVAP.gw	Groundwater “revap” coefficient		0.02–0.2	0.08
GW_SPYLD.gw	Special yield of the shallow aquifer	m ³ m ⁻³	0–0.4	0.13
GWHT.gw	Initial groundwater height	m	0–25	14
GWQMN.gw	Threshold depth of water in the shallow aquifer required for return flow to occur	mm	0–5000	372
RCHRG_DP.gw	Deep aquifer percolation fraction		0–1	0.87
REVAPMN.gw	Threshold depth of water in the shallow aquifer required for “revap” to occur	mm	0–500	260
CANMX.hru	Maximum canopy storage	mm	0–100	0.6
EPCO.hru	Plant uptake compensation factor		0–1	0.34
ESCO.hru	Soil evaporation compensation factor		0–1	0.9
HRU_SLP.hru	Average slope steepness	m m ⁻¹	0–0.6	0.5
LAT_TTIME.hru	Lateral flow travel time	d	0–180	3
RSDIN.hru	Initial residue cover	kg ha ⁻¹	0–10000	1
SLSOIL.hru	Slope length for lateral subsurface flow	m	0–150	40
CH_K2.rte	Effective hydraulic conductivity in the main channel alluvium	mm h ⁻¹	0–500	20
CH_N2.rte	Manning's N value for the main channel		0–0.3	0.16

CH_K1.sub	Effective hydraulic conductivity in the tributary channel alluvium	mm h ⁻¹	0–300	100
CH_N1.sub	Manning's N value for the tributary channel		0.01–30	20
SS				
USLE_P.mgt	USLE equation support practice factor		0–1	0.5
PRF.bsn	Peak rate adjustment factor for sediment routing in the main channel		0–2	1.9
SPCON.bsn	Linear parameter for calculating the maximum amount of sediment that can be re-entrained during channel sediment routing		0.0001–0.01	0.001
SPEXP.bsn	Exponent parameter for calculating sediment re-entrained in channel sediment routing		1–1.5	1.26
LAT_SED.hru	Sediment concentration in lateral flow and groundwater flow	mg L ⁻¹	0–5000	5.7
OV_N.hru	Manning's N value for overland flow		0.01–30	28
SLSUBBSN.hru	Average slope length	m	10–150	92
CH_COV1.rte	Channel erodibility factor		0–0.6	0.17
CH_COV2.rte	Channel cover factor		0–1	0.6
TP				
P_UPDIS.bsn	Phosphorus uptake distribution parameter		0–100	0.5
PHOSKD.bsn	Phosphorus soil partitioning coefficient		100–200	174
PPERCO.bsn	Phosphorus percolation coefficient		10–17.5	14
PSP.bsn	Phosphorus sorption coefficient		0.01–0.7	0.5
GWSOLP.gw	Soluble phosphorus concentration in groundwater loading	mg P L ⁻¹	0–1000	0.063
LAT_ORGP.gw	Organic phosphorus in the base flow	mg P L ⁻¹	0–200	0.01
ERORGP.hru	Organic phosphorus enrichment ratio		0–5	2.5
CH_OPCO.rte	Organic phosphorus concentration in the channel	mg P L ⁻¹	0–100	0.02
BC4.swq	Rate constant for mineralization of organic phosphorus to dissolved phosphorus in the reach at 20 °C	d ⁻¹	0.01–0.7	0.3
RS2.swq	Benthic (sediment) source rate for dissolved phosphorus in the reach at 20 °C	mg m ⁻² d ⁻¹	0.001–0.1	0.02
RS5.swq	Organic phosphorus settling rate in the reach at 20 °C	d ⁻¹	0.001–0.1	0.05

TN				
RSDCO.bsn	Residue decomposition coefficient		0.02–0.1	0.09
CDN.bsn	Denitrification exponential rate coefficient		0–3	0.3
CMN.bsn	Rate factor for humus mineralization of active organic nitrogen		0.001–0.003	0.002
N_UPDIS.bsn	Nitrogen uptake distribution parameter		0–100	0.5
NPERCO.bsn	Nitrogen percolation coefficient		0–1	0.0003
RCN.bsn	Concentration of nitrogen in rainfall	mg N L ⁻¹	0–15	0.34
SDNCO.bsn	Denitrification threshold water content		0–1	0.02
HLIFE_NGW.gw	Half-life of nitrate–nitrogen in the shallow aquifer	d	0–200	195
LAT_ORGN.gw	Organic nitrogen in the base flow	mg N L ⁻¹	0–200	0.055
SHALLST_N.gw	Nitrate–nitrogen concentration in the shallow aquifer	mg N L ⁻¹	0–1000	1
ERORGN.hru	Organic nitrogen enrichment ratio		0–5	3
CH_ONCO.rte	Organic nitrogen concentration in the channel	mg N L ⁻¹	0–100	0.01
BC1.swq	Rate constant for biological oxidation of ammonium–nitrogen to nitrite–nitrogen in the reach at 20 °C	d ⁻¹	0.1–1	1
BC2.swq	Rate constant for biological oxidation of nitrite–nitrogen to nitrate–nitrogen in the reach at 20 °C	d ⁻¹	0.2–2	0.7
BC3.swq	Rate constant for hydrolysis of organic nitrogen to ammonium–nitrogen in the reach at 20 °C	d ⁻¹	0.2–0.4	0.4
RS3.swq	Benthic (sediment) source rate for ammonium–nitrogen in the reach at 20 °C	mg m ⁻² d ⁻¹	0–1	0.2
RS4.swq	Rate coefficient for organic nitrogen settling in the reach at 20 °C	d ⁻¹	0.001–0.1	0.05

1 Table 5. Criteria for model performance. Note: o_n is the n^{th} observed datum, s_n is the n^{th} simulated datum, \bar{o} is the observed mean
2 value, \bar{s} is the simulated daily mean value, and N is the total number of observed data. Performance rating criteria are based on
3 Moriasi et al. (2007) for Q: discharge, SS: suspended sediment, TP: total phosphorus and TN: total nitrogen. Moriasi et al. (2007)
4 derived these criteria based on extensive literature review and analysing the reported performance ratings for recommended model
5 evaluation statistics.

Statistic equation	Constituent	Performance ratings			
		Unsatisfactory	Satisfactory	Good	Very good
$R^2 = \frac{\{\sum_{n=1}^N [(s_n - \bar{s})(o_n - \bar{o})]\}^2}{\sum_{n=1}^N (o_n - \bar{o})^2 \times \sum_{n=1}^N (s_n - \bar{s})^2}$ (3)	All	< 0.5	0.5 – 0.6	0.6 – 0.7	0.7 – 1
$NSE = 1 - \frac{\sum_{n=1}^N (o_n - s_n)^i}{\sum_{n=1}^N (o_n - \bar{o})^i}$ $i = 2$ (4)	All	< 0.5	0.5 – 0.65	0.65 – 0.75	0.75 – 1
$\pm \text{PBIAS}\% = \frac{\sum_{n=1}^N (o_n - s_n)}{\sum_{n=1}^N o_n} \times 100$ (5)	Q	> 25	15 – 25	10 – 15	< 10
	SS	> 55	30 – 55	15 – 30	< 15
	TP, TN	> 70	40 – 70	25 – 40	< 25

6 R^2 : coefficient of determination

7 NSE: Nash–Sutcliffe efficiency

8 PBIAS: percent bias

- 1 Table 6. Model performance ratings for simulations of discharge (Q), concentrations of suspended sediment (SS), total phosphorus
2 (TP) and total nitrogen (TN). n indicates the number of measurements. Q-weighted mean concentrations were calculated using Eq.
3 (1).

Model performance	Statistics	Q	SS	TP	TN
		n = 1439	n = 43	n = 45	n = 39
Calibration with instantaneous measurements (2004–2008)	R ²	0.77 (Very good)	0.42 (Unsatisfactory)	0.02 (Unsatisfactory)	0.08 (Unsatisfactory)
	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)
		n = 1294	n = 37	n = 37	n = 36
Validation with instantaneous measurements (1994–1997)	R ²	0.68 (Good)	0.80 (Very good)	0.01 (Unsatisfactory)	0.01 (Unsatisfactory)
	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)
		–	n = 12	n = 18	n = 18
Validation with Q-weighted mean concentrations (2010–2012)	R ²	–	0.38 (Unsatisfactory)	0.06 (Unsatisfactory)	0.46 (Unsatisfactory)
	NSE	–	-0.03 (Unsatisfactory)	-4.88 (Unsatisfactory)	0.42 (Unsatisfactory)
	±PBIAS%	–	43.9 (Satisfactory)	69.4 (Satisfactory)	-0.87 (Very good)

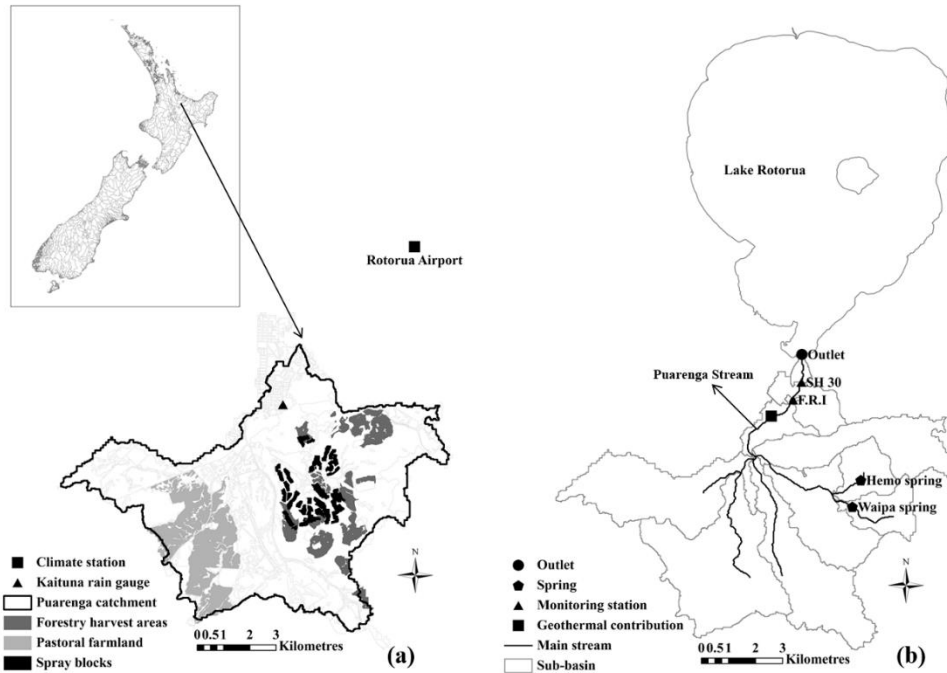
- 1 Table 7. Model performance statistics for simulations of discharge (Q), and loads of suspended sediment (SS), total phosphorus (TP) and total
2 nitrogen (TN). Statistics were calculated for both overall and separated simulations. Q_{all} and L_{all} indicate the overall simulations; Q_b and L_b
3 indicate the base flow simulations; Q_q and L_q indicate the quick flow simulations.

Model performance	Statistics	Q			SS			TP			TN		
		Q_b	Q_q	Q_{all}	L_b	L_q	L_{all}	L_b	L_q	L_{all}	L_b	L_q	L_{all}
Calibration (2004–2008)	R^2	0.84	0.84	0.77	0.66	0.68	0.61	0.24	0.65	0.39	0.72	0.97	0.95
	NSE	0.6	0.71	0.73	0.33	0.33	0.27	-6.2	0.09	-0.17	0.5	0.89	0.85
	\pm PBIAS%	7.5	8.7	7.8	7.57	-23.4	-3.6	45.4	40.1	43.6	0.8	6.6	2.7
Validation (1994–1997)	R^2	0.87	0.81	0.68	0.36	0.98	0.95	0.27	0.27	0.06	0.79	0.33	0.58
	NSE	0.56	0.62	0.62	-0.03	0.43	0.85	-1.9	0.04	-0.64	0.58	-0.07	0.33
	\pm PBIAS%	11.3	-1.2	8.8	34.5	-79.7	11.1	45.8	-9.3	37	-7.6	14.3	-2.5

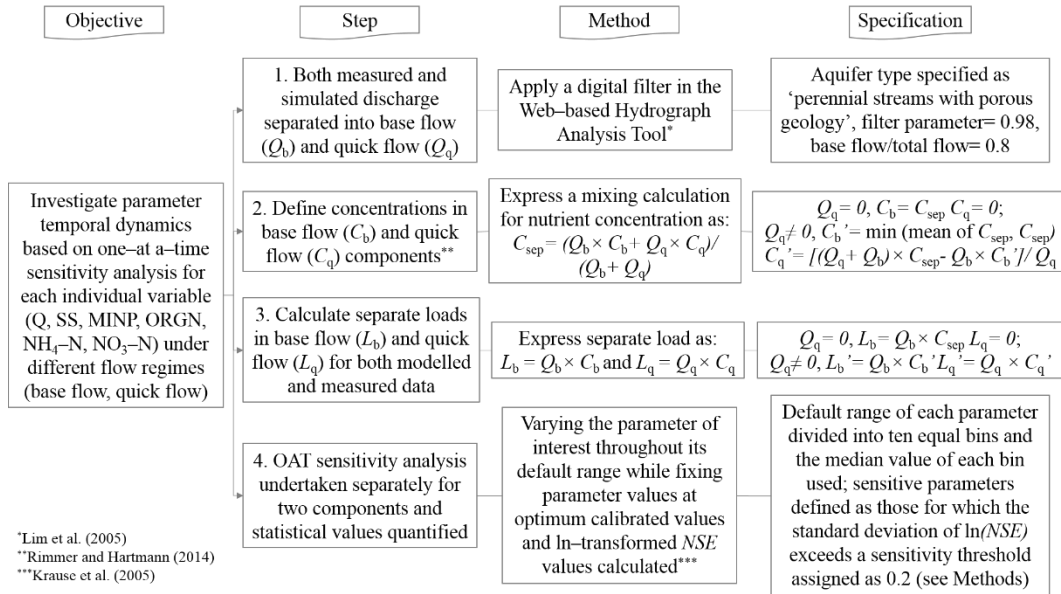
- 4 R^2 : coefficient of determination; NSE: Nash–Sutcliffe efficiency; PBIAS: percent bias

1 Table 8 Rankings of relative sensitivities of parameters (from most to least) for variables (header row) of Q (discharge), SS (suspended sediment),
2 MINP (mineral phosphorus), ORGN (organic nitrogen), NH₄-N (ammonium-nitrogen), and NO₃-N (nitrate-nitrogen). Relative sensitivities
3 were identified by randomly generating combinations of values for model parameters and comparing modelled and measured data with a
4 Student's t test ($p \leq 0.05$). Bold text denotes that a parameter was deemed sensitive relative to more than one simulated variable. Shaded text
5 denotes that parameter deemed insensitive to any of the two flow components (base and quick flow; see Figure 7) using one-at-a-time sensitivity
6 analysis. Definitions and units for each parameter are shown in Table 4.

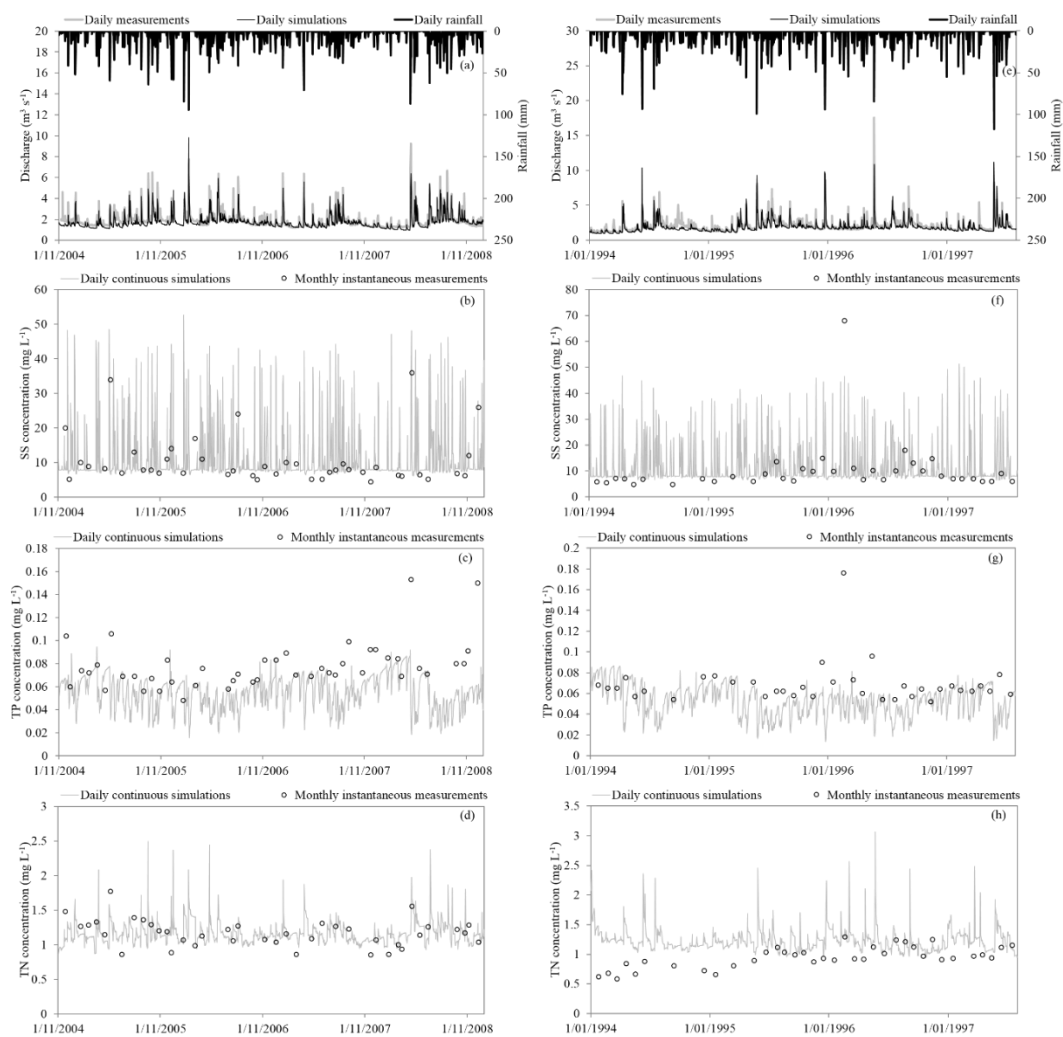
Q	SS	MINP	ORGN	NH ₄ -N	NO ₃ -N
SLSOIL	LAT_SED	CH_OPCO	CH_ONCO	CH_ONCO	NPERCO
CH_K2	CH_N2	BC4	BC3	BC1	CDN
HRU_SLP	SLSUBBSN	RS5	SOL_CBN(1)	CDN	ERORGN
LAT_TTIME	SPCON	ERORGP	RS4	RS3	CMN
SOL_AWC(1)	ESCO	PPERCO	RCN	RCN	RCN
RCHRG_DP	OV_N	RS2	N_UPDIS		RSDCO
GWQMN	SLSOIL	PHOSKD	USLE_P		
GW_REVAP	LAT_TTIME	GWSOLP	SDNCO		
GW_DELAY	SOL_AWC(1)	LAT_ORGP	SOL_NO3(1)		
CH_COV1	EPCO		CMN		
CH_COV2	CANMX		HLIFE_NGW		
EPCO	CH_K2		RSDCO		
SPEXP	GW_DELAY		USLE_K(1)		
CANMX	ALPHA_BF				
CH_N1	GW_REVAP				
PRF	CH_COV1				
SURLAG					



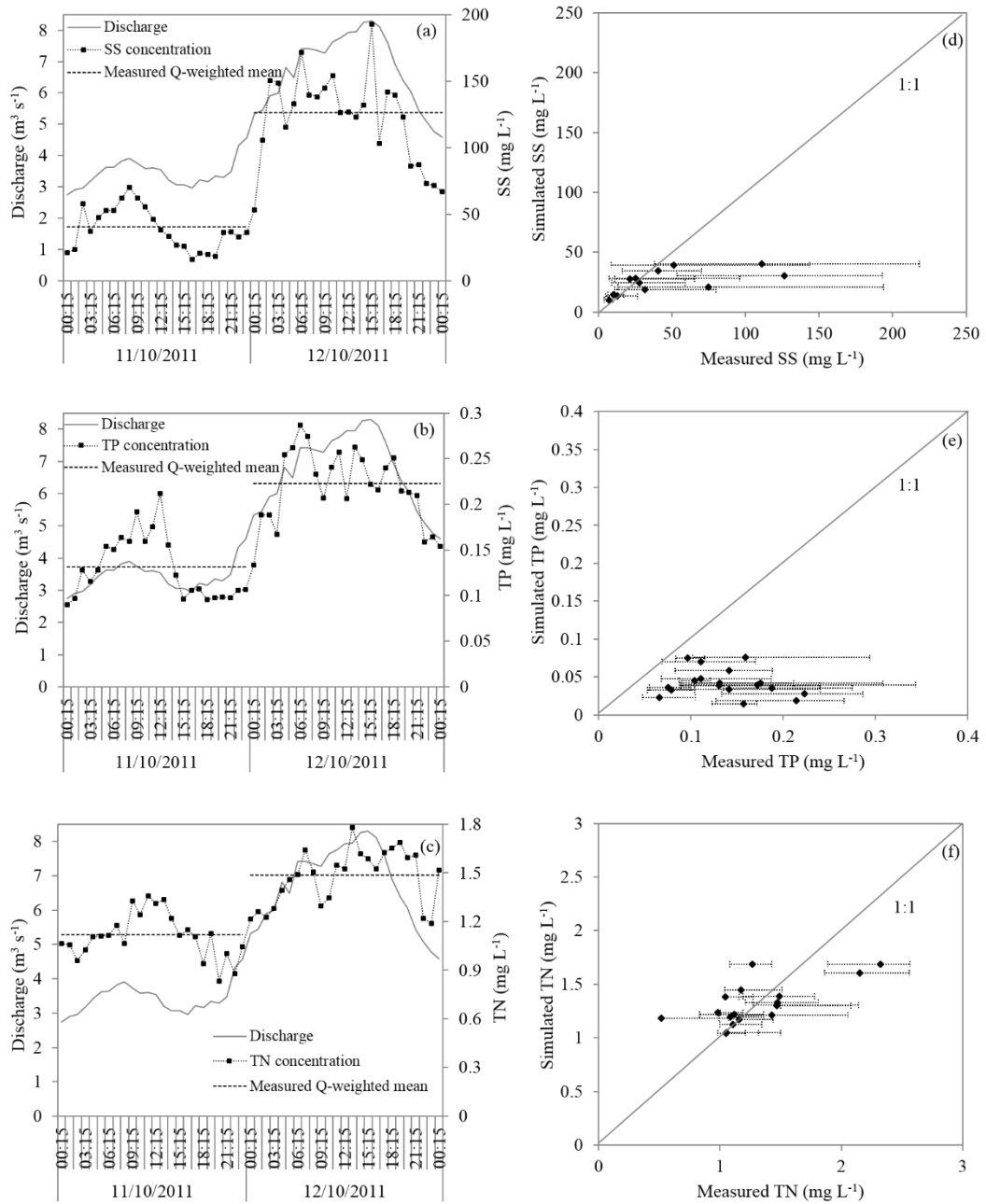
1
 2 Figure 1. (a) Location of Puarenga Stream surface catchment in New Zealand,
 3 Kaituna rain gauge, climate station and managed land areas for which
 4 management schedules were prescribed in SWAT, and (b) location of the
 5 Puarenga Stream, major tributaries, monitoring stream-gauges, two cold-water
 6 springs and the Whakarewarewa geothermal contribution. Measurement data
 7 (Table 3) used to calibrate the SWAT model were from the Forest Research
 8 Institute (FRI) stream-gauge and were considered representative of the
 9 downstream/outlet conditions of the Puarenga Stream.



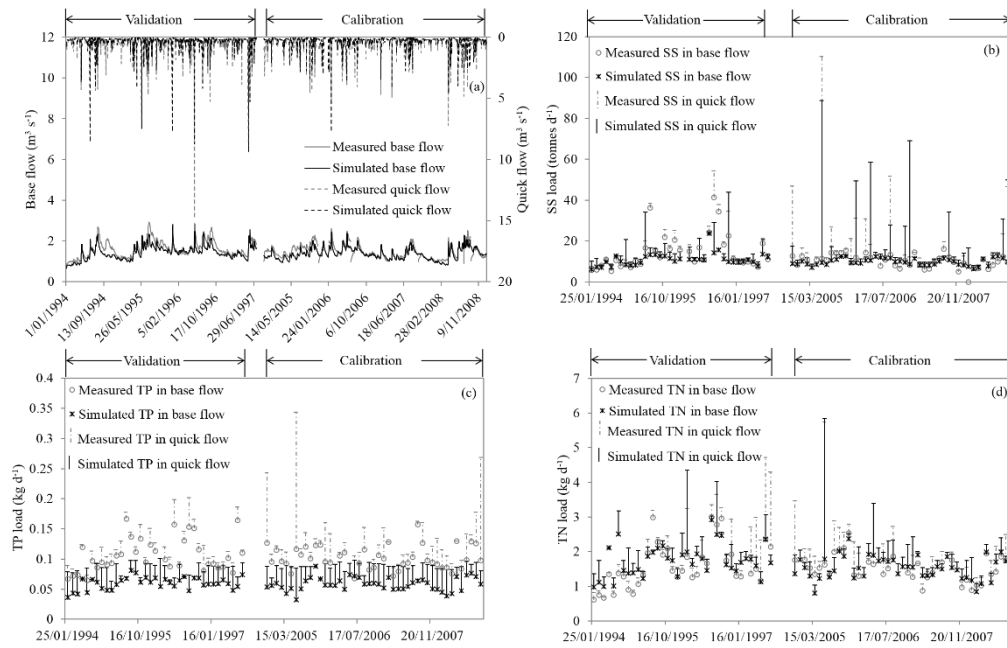
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2 Figure 2. Flow chart of methods used to separate hydrograph and contaminant
3 loads and to quantify parameter sensitivities for: Q (discharge), SS (suspended
4 sediment), MINP (mineral phosphorus), ORGN (organic nitrogen), NH₄-N
5 (ammonium-nitrogen), and NO₃-N (nitrate-nitrogen). NSE : Nash-Sutcliffe
6 efficiency.



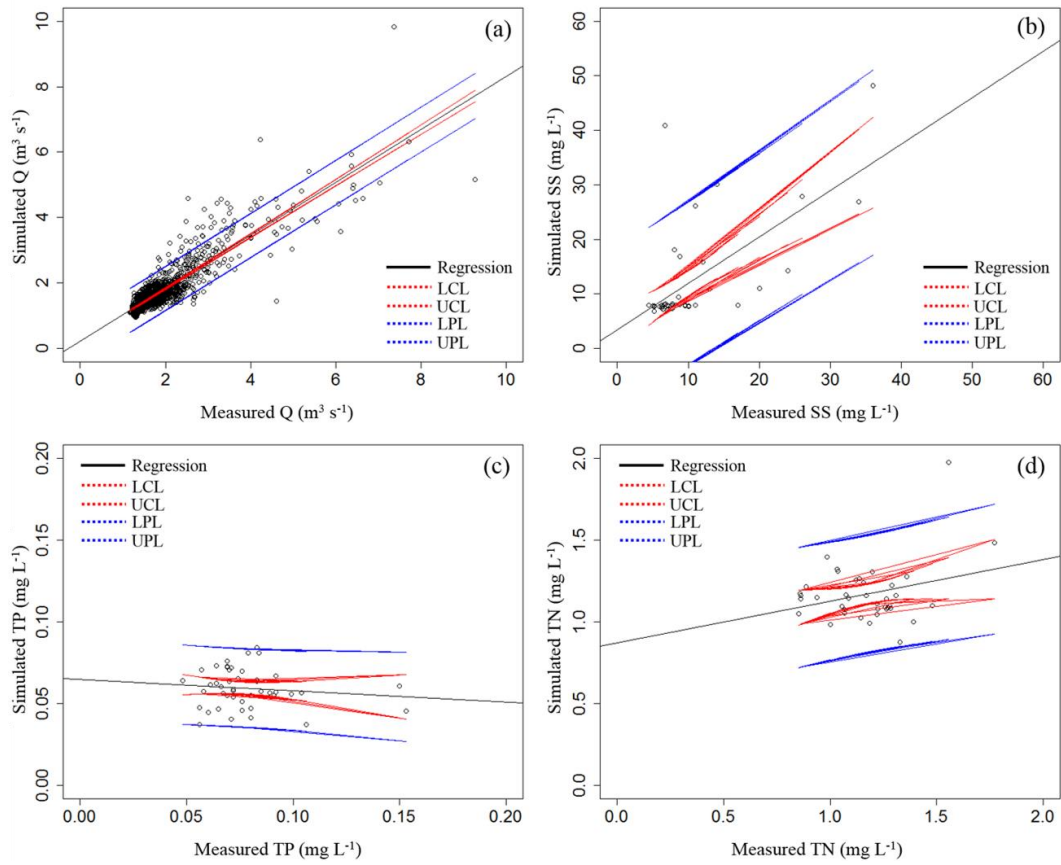
1
 2 Figure 3. Measurements and daily mean simulated values of discharge, suspended
 3 sediment (SS), total phosphorus (TP) and total nitrogen (TN) during calibration
 4 (a–d) and validation (e–h). Measured daily mean discharge was calculated from
 5 15-min observations and measured concentrations of SS, TP and TN correspond
 6 to monthly grab samples.



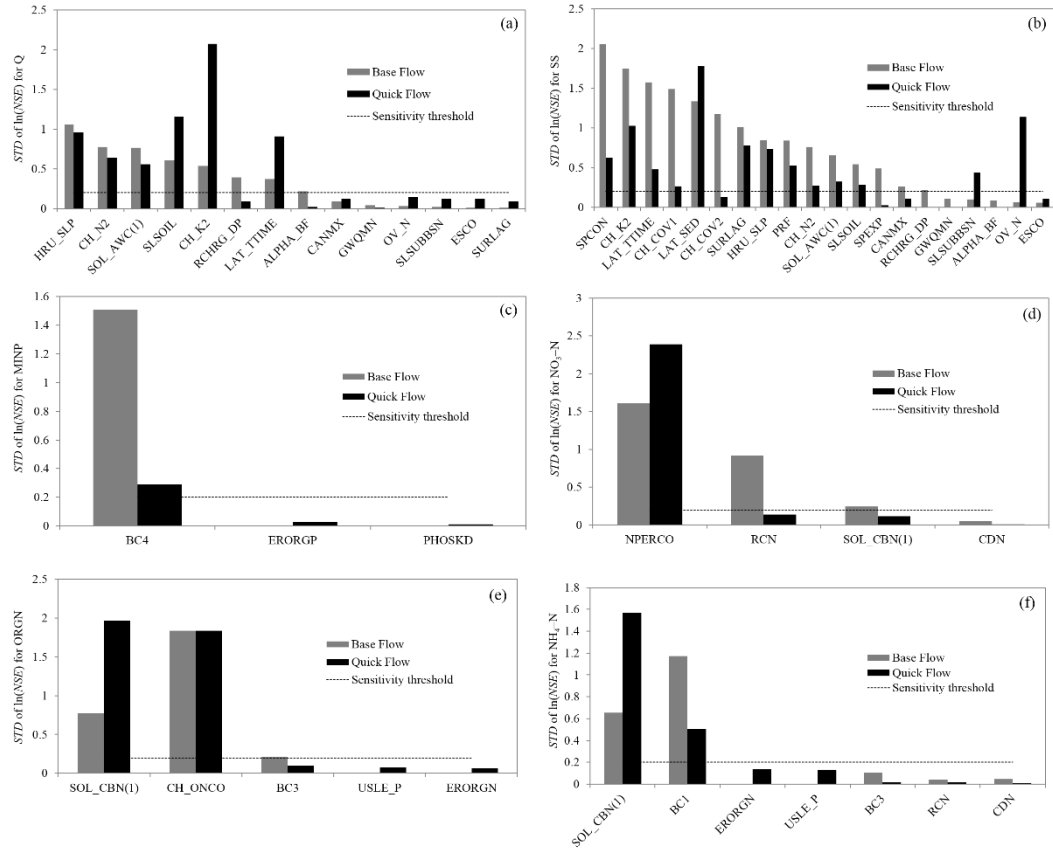
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2 Figure 4. Example of a storm event showing derivation of discharge (Q)-weighted
3 daily mean concentrations (dashed horizontal line) based on hourly measured
4 concentrations (black dots) of suspended sediment (SS), total phosphorus (TP)
5 and total nitrogen (TN) over two days (a–c). Comparisons of Q-weighted daily
6 mean concentrations with simulated daily mean estimates of SS, TP and TN
7 (scatter plot, d–f). The horizontal bars show the ranges in hourly measurements
8 during each storm event in 2010–2012.



1
 2 Figure 5. Measurements and simulations derived using the calibrated set of
 3 parameter values. Data are shown separately for base flow and quick flow. (a)
 4 Daily mean base flow and quick flow; (b) suspended sediment (SS) load; (c) total
 5 phosphorus (TP) load; (d) total nitrogen (TN) load. Vertical lines in b–d show the
 6 contaminant load in quick flow. Time series relate to calibration (2004–2008) and
 7 validation (1994–1997) periods (note time discontinuity). Measured instantaneous
 8 loads of SS, TP, and TN correspond to monthly grab samples.



1
 2 Figure 6. Regression of measured and simulated (a) discharge (Q), concentrations
 3 of (b) suspended sediment (SS), (c) total phosphorus (TP), and (d) total nitrogen
 4 (TN) including lower and upper 95% confidence limits (LCL and UCL) and lower
 5 and upper 95% prediction limits (LPL and UPL). Note that the “choppy” shape of
 6 confidence limits shown in figures b–d resulted from the few data points (< 50) in
 7 the regressions of measured and simulated SS, TP and TN concentrations.



1
2 Figure 7. The standard deviation (STD) of the ln-transformed Nash-Sutcliffe
3 efficiency (NSE) used to indicate parameter sensitivity based on one-at-a-time
4 (OAT) sensitivity analysis for separate base and quick flow components: (a) Q
5 (discharge); (b) SS (suspended sediment); (c) MINP (mineral phosphorus); (d)
6 NO₃-N (nitrate-nitrogen); (e) ORGN (organic nitrogen); (f) NH₄-N (ammonium-
7 nitrogen). A median value (0.2) derived from the STD of ln-transformed NSE was
8 chosen as a threshold above which parameters were deemed to be 'sensitive'.
9 Definitions of each parameter are shown in Table 4.