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USING MONTHLY STREAM WATER QUALITY DATA TO QUANTIFY NITRATE TRANSFER PATHWAYS IN THREE WAIKATO CATCHMENTS

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Abstract

Monthly water quality sampling at the catchment outlet is carried out at many sites across New Zealand for state of the environment monitoring. This data is used for trend analysis, but little else. We have been exploring approaches for using this data in conjunction with concurrent stream flow data to identify and quantify the principal nutrient transfer pathways within catchments. In particular, monthly data may provide sufficient information for an inverse modelling approach.

Three contrasting mesoscale catchments were chosen for this study: (1) the Tahunaatara Stream (208 km^2) in the Upper Waikato subregion, (2) the Puniu River (519 km^2) in the Waipa subregion, and (3) the Mangatangi River (195 km^2) in the Lower Waikato subregion. By considering four years of monthly water quality data from these catchments, alongside daily rainfall, potential evapotranspiration, and stream flow measurements, we were able to use the daily time step, spatially lumped catchment model “StreamGEM” with the Markov Chain Monte Carlo algorithm “DREAM$_{ZS}$” to predict daily stream flow and nitrate fluxes arriving at the catchment outlet via near-surface (NS), shallow fast seasonal groundwater (F), and deep slow older groundwater (S) flow paths, as well as to estimate the reliability/uncertainty of these predictions.

Despite high uncertainty in some model parameters, the flow and nitrate calibration data was well reproduced across all catchments (Nash-Sutcliffe model efficiency in the range 0.70–0.83 for daily flow, and 0.17–0.88 for nitrate concentration, both on log scale). Proportions of flow attributed to near-surface, fast seasonal groundwater and slow older groundwater were well defined, and consistent with expectations based on catchment geology. Fast groundwater contributed the bulk of the annual average nitrate yield in all of these catchments (range 31–97%), although contributions from slow groundwater were also high at Tahunaatara (range 18–63%), while contributions from near-surface flow were high at Mangatangi (range 24–63%).

This research highlights the potential of process based, spatially lumped modelling with commonly available monthly stream sample data, to elucidate high resolution catchment function, when appropriate calibration methods are used that correctly handle the inherent uncertainties.

Introduction

Waikato Regional Council has been collecting monthly grab samples at 114 sites across the region since the early 1990s for the purpose of river water quality monitoring (WRC, 2013). These data are typically used only for state of the environment reporting and trend analysis. We have been interested in whether additional insight into nutrient transfer pathways can be gleaned by incorporating stream flow data into the analysis of the water quality data. Twentysix monitoring sites were identified at which high resolution stream flow records (typically 15-minute) were available at or near the water quality monitoring location (Fig. 1), and a preliminary study looked at simple options for analysing this data (Woodward, 2015; Woodward et al., 2016a).

The current study extends this by applying the "StreamGEM" inverse modelling approach, which was developed for the small (15 km^2) Toenepi dairying catchment near Morrinsville (Fig. 1; Bidwell et al., 2008; Woodward et al., 2013), to three contrasting, larger catchments. The StreamGEM approach uses calibration of a simple, physically-based, spatially-lumped catchment model to stream flow and nitrate data simultaneously, to determine the key catchment hydrological and chemical parameters and their uncertainty. The calibrated model can then be used to make predictions of catchment function: for example flow path partitioning on a daily basis, or annual average nitrate fluxes.

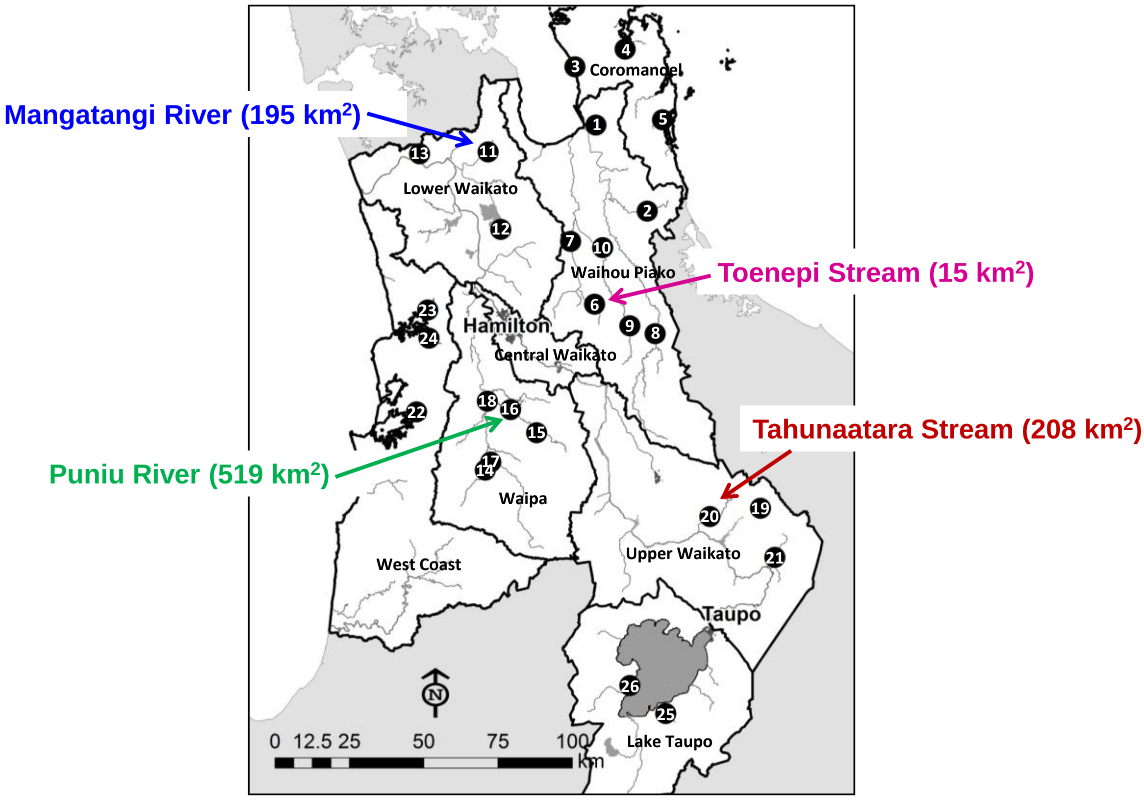


Figure 1: Waikato Region, showing 26 water quality monitoring sites where flow data is also available, and delineation of major subregions. The StreamGEM model was developed for the Toenepi Stream catchment (near 6). Catchments studied in this paper are the Tahunaatara Stream (20), Puniu River (16) and Mangatangi River (11).

Materials and Methods

Catchment Data

The three catchments selected for this study were the Tahunaatara Stream (208 km^2), in the porous, pumiceous uplands of the Lake Taupo volcanic zone, the Puniu River (519 km^2), in the loamy, allophanic lowlands of the Waipa district, and the Mangatangi River (195 km^2), in the clayey, granular foothills of the Hunua Ranges in the Lower Waikato subregion (Fig. 1). Land use intensity is similar between the catchments, with a mixture of dairy, drystock and native forest. There is also a significant area of exotic forestry in the uplands of the Tahunaatara catchment.

The four year period 1 April 2003 to 30 March 2007 was chosen for model calibration, and daily stream flow (normalised over catchment area as mm d^{-1}) and monthly stream nitrate concentrations (measured as mg nitrate-nitrite nitrogen L^{-1}, although nitrite concentrations were negligible) were assembled for each catchment. Daily rainfall and potential evapotranspiration (PET) were also obtained from NIWA climate stations near each catchment (up to 40 km away), and these were adjusted using a rainfall scaling parameter to account for orographic effects. Further details of the catchment data can be found in Woodward et al. (2016b).

Hydrological Model

Use of a hydrological model is a way to add process understanding into the analysis of catchment data. The hydrological equations and parameters constrain the modelled catchment response so that the real world data is interpreted in a physically meaningful way. The calibrated model parameter values, and subsequent model predictions, are then more likely to be realistic and reliable.

Fig. 2 shows the input and output data used by the StreamGEM model (Woodward et al., 2013, 2016b), and the water reservoirs and flow paths simulated. Daily rainfall and potential evapotranspiration (PET) inputs are used to drive near-surface runoff prediction and a daily soil water balance. Excess soil water percolates through the vadose zone to recharge groundwater, and two groundwater reservoirs are considered, one consisting of fast, shallow groundwater, and the other of slow, deeper groundwater. The groundwater reservoirs are modelled using a linearised Boussinesq equation to represent water table slope and discharge. This gives a total of three flow paths discharging to the stream, which as an approximation are assumed to have constant nitrate concentrations. The “end-member mixing” assumption then assumes that day to day changes in stream nitrate concentration are solely due to changes in the relative contributions of the three flow paths. Concentration changes within flow paths, e.g. due to land use changes or water table fluctuations, are not currently modelled: adding too much process detail without sufficient calibration information to support it can reduce a model’s predictive usefulness. Nevertheless these details will need to be addressed in future.

The StreamGEM model has a total of 13 adjustable parameters representing the hydrological behaviour of the the catchment and the nitrate concentrations in the discharge flow paths, and these are estimated by calibration to the observed catchment data, as follows.

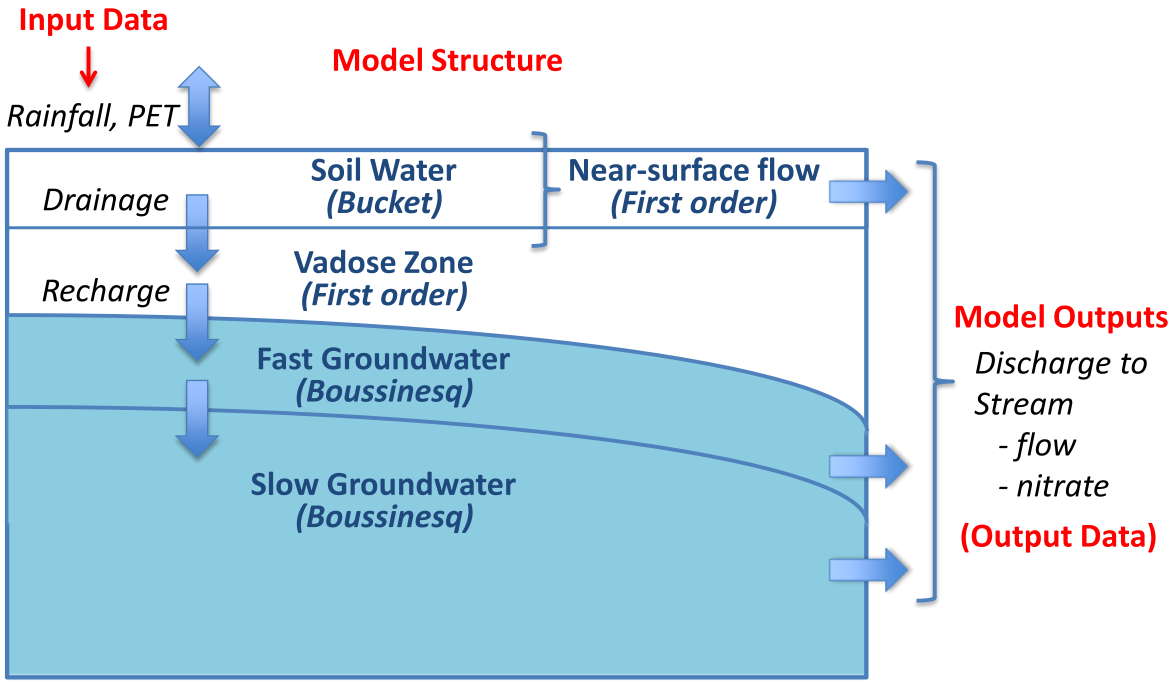


Figure 2: Catchment hydrological processes, water reservoirs and flow paths simulated in the StreamGEM model ("Streamflow Generation Eigen-Model"). The model has 13 parameters, representing the catchment hydrological characteristics, that are determined by calibration.

Calibration Method

Model calibration was carried out using the Markov Chain Monte Carlo method, as implemented in the DREAM$_{ZS}$ code (ter Braak & Vrugt, 2008). This method uses Bayesian statistical theory to estimate the posterior distribution of the parameters, i.e., the collection of model parameter sets for which the given data (stream flow and nitrate simultaneously) can be considered a likely sample. Importantly, the approach calculates not only the maximum likelihood (ML) parameter set, but also the uncertainty, as represented by the range of parameter sets that fit the data. Uncertainty describes our lack of knowledge about a quantity of interest, which is different from *variation*, which describes how a known measurement changes over time or space or between individuals. Uncertainty in model predictions exists because of the inherent uncertainty in the data values, uncertainty about the model structure, and uncertainty about the measurement errors.

We generated a posterior distribution with 10000 parameter sets, and discarded the least likely 5%, leaving 9500 parameter sets. Finally, these parameter sets were used to calculate model predictions, both maximum likelihood values and their uncertainty.

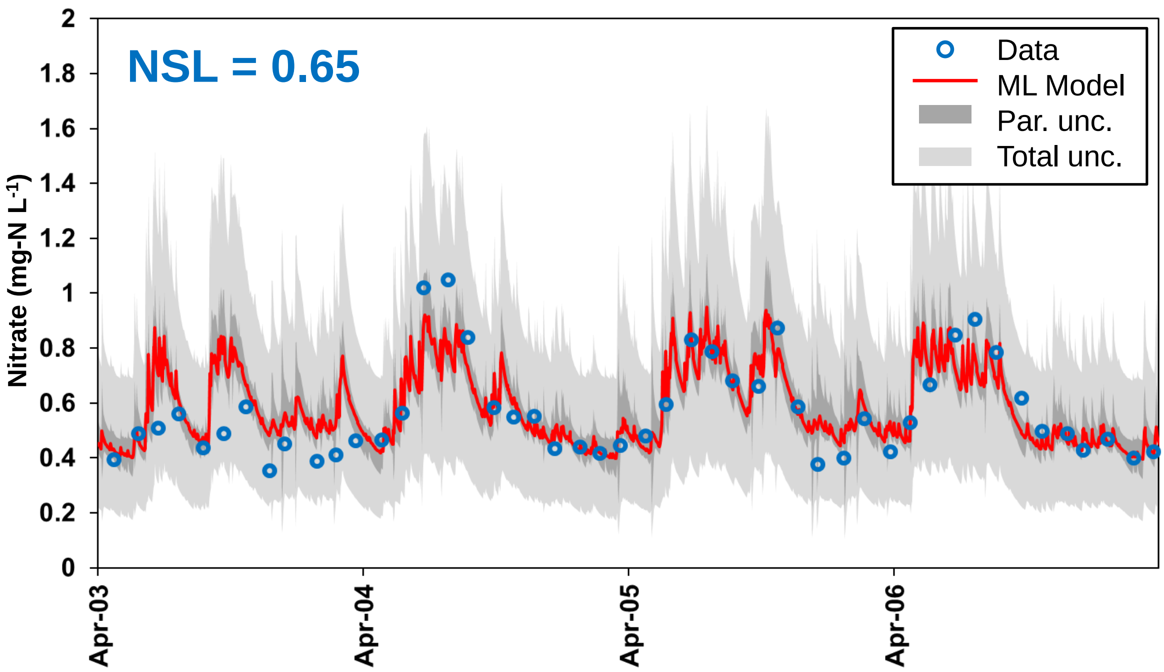
Results

Results of the calibration included distributions for the calibration metrics (e.g. likelihood, Nash-Sutcliffe values), model parameters (e.g. flow path hydrological response times and discharge concentrations), and model predictions (e.g. annual average water and nitrate fluxes from each flow path). The current paper focuses on selected results only; the full analysis is presented in Woodward et al. (2016b).

Goodness of Fit Check

Before looking at the predictions, it is important to check the calibration. If the calibrated model does not give a good fit to the data, other predictions are unlikely to be reliable. For example, Fig. 3 shows the calibration of the model to the four years of stream nitrate and flow data from the Tahunaatara Stream monitoring site. As well as the measured data, the figure shows the daily nitrate and flow predictions from the maximum likelihood parameter set (in red), and from all of the 9500 posterior parameter sets ("Par. unc.") in dark grey. The narrow band of dark grey shows that all of the posterior parameter sets gave a similarly good fit to the data. The total uncertainty ("Total unc.") is also shown in light grey, and illustrates the possible effect of measurement and model structure error. Calculating the familiar Nash-Sutcliffe model efficiency (NSL, calculated on log scale) for each posterior parameter set showed that the flow and nitrate calibration data was well reproduced across all three catchments, with NSL in the range 0.70–0.83 for daily flow, and 0.17–0.88 for monthly nitrate. The lowest values of NSL for nitrate reflect the small variability in the nitrate concentrations at Tahunaatara.

(a)



(b)

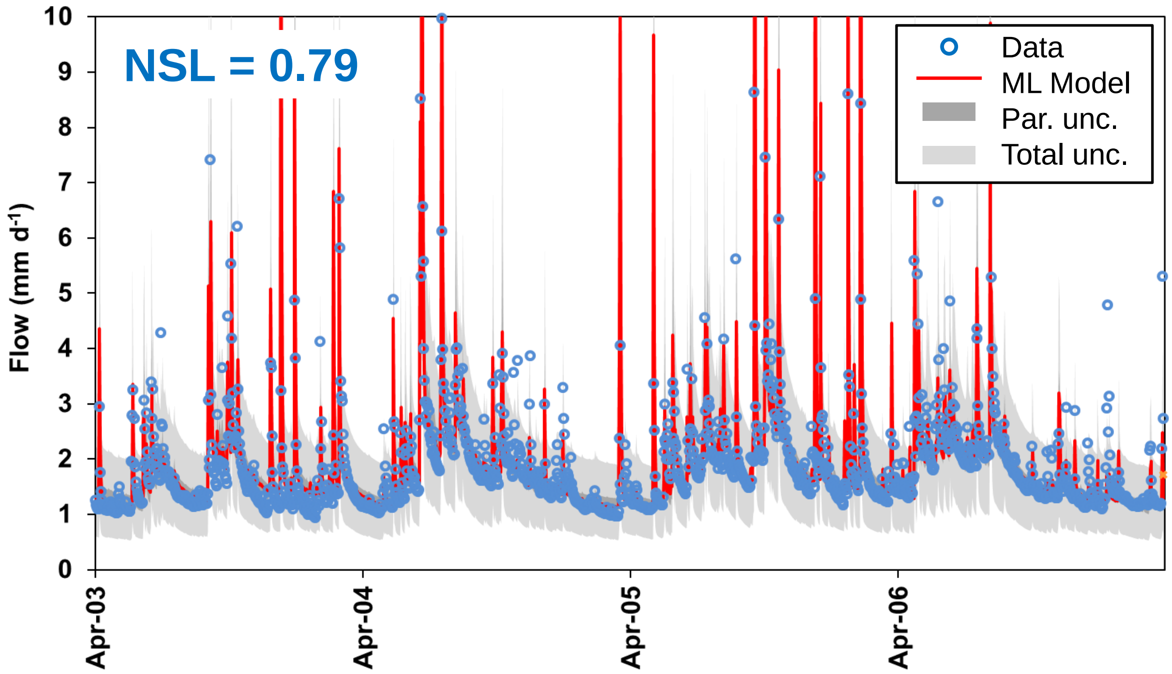


Figure 3: Example of model calibration, to four years of (a) monthly stream nitrate and (b) daily stream flow data from the Tahunaatara Stream. Nash-Sutcliffe model efficiency against the log transformed data (NSL) of the maximum likelihood (ML) model is also shown. Parameter uncertainty and total uncertainty are described in the text.

Predictions

The model was then used to predict several catchment fluxes of interest, using each of the best 9500 parameter sets that gave a good fit to the data. The range/uncertainty of these predictions is typically greater than the uncertainty of the calibration which is constrained directly by observations. Indeed the uncertainty can be quite large, particularly where there is a weak correlation between the calibration data and the prediction of interest.

Fig. 3 presents three predictions selected for this paper. The predictions are presented as boxplots, which show the median, upper and lower quartiles, and range of the predicted values across the parameter sets. The maximum likelihood value is also shown; this has no particular reliability, but is analogous to the single "best fit" predictions presented in other studies. Full results are presented in Woodward et al. (2016b).

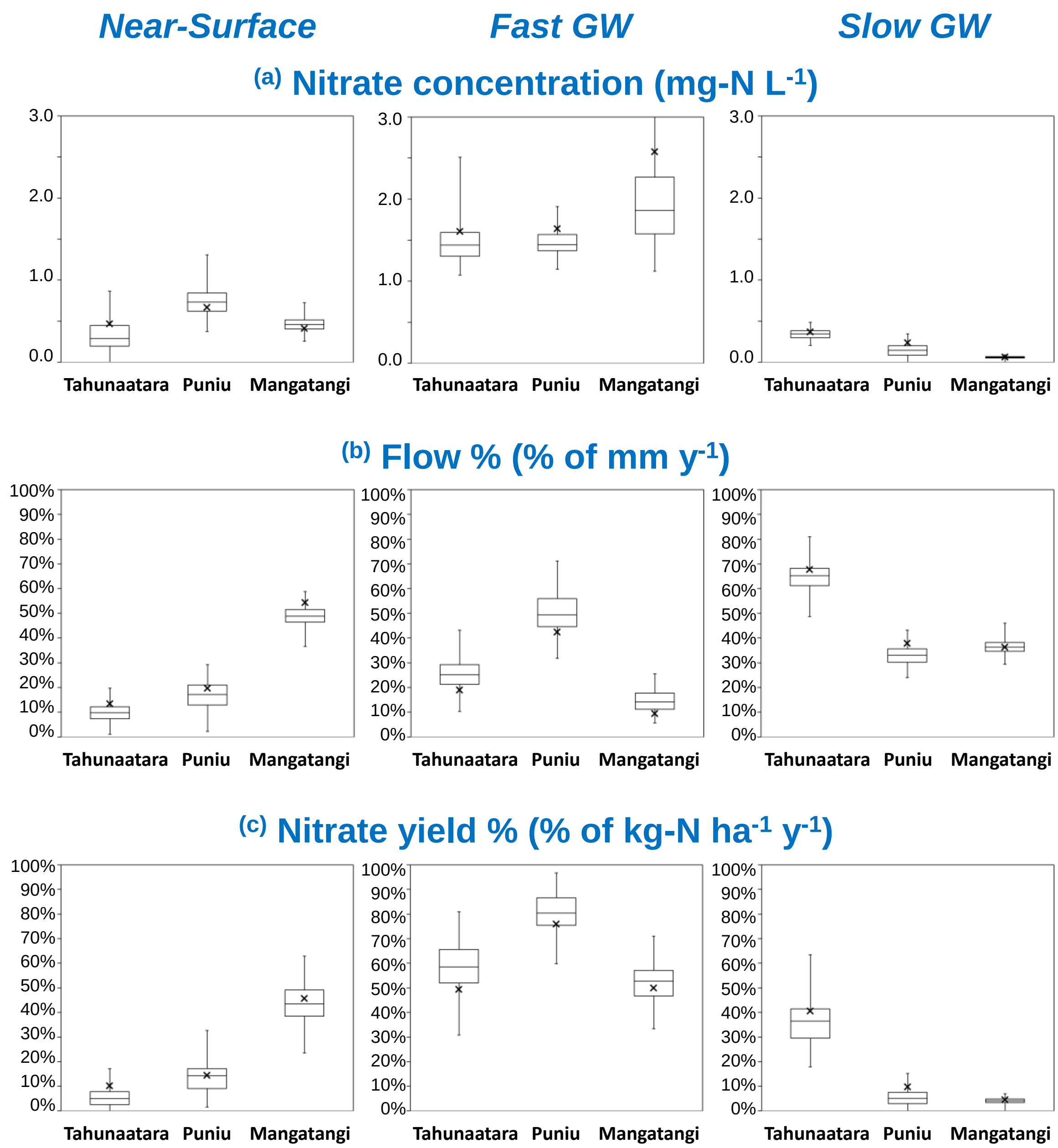


Figure 4: Model predictions of flow path (a) nitrate concentration, (b) annual average water flux, and (c) annual average nitrate flux, for water discharged from near surface, fast groundwater and slow groundwater flow paths respectively, for the three catchments. 'X' shows the maximum likelihood value, and boxplots show the quartiles and ranges of the 9500 most likely parameter sets.

The first row of Fig. 3 shows the predicted values of the model parameters that represent the nitrate concentrations in water discharged into the stream from the near-surface, fast groundwater and slow groundwater flow paths respectively. The concentrations are reasonably well defined (moderate uncertainty), and distinct between flow paths. They are also similar between the three catchments studied here (0.0-1.3 mg-N L^{-1} for near-surface, 1.1-4.3 mg-N L^{-1} for fast groundwater and 0.0-0.5 mg-N L^{-1} for slow groundwater), possibly reflecting the similar land use intensity between the catchments. The lower concentrations in near surface flow are probably due to dilution effects during storm flow, while the lower concentrations in slow groundwater may reflect older water recharged prior to land use intensification, or subsurface denitrification, which may be relatively widespread in this region (Close et al. 2016).

Annual average stream flow was predicted to be 662-789 mm y^{-1} at Tahunaatara, 886-1062 mm y^{-1} at Puniu, and 457-531 mm y^{-1} at Mangatangi. The second row of Fig. 3 shows the predicted contribution to this flow from each of the three flow paths (% of mm y^{-1}). Again, the predictions are reasonably well defined, and we now observe important differences between the three catchments. In particular, near-surface flow contributes much more discharge in the Mangatangi catchment (36-59%) compared with the other catchments (1-29%), while slow groundwater contributes much more in the Tahunaatara catchment (49-81%) compared with the others (24-46%). These observations match our knowledge of catchment geology, with the clay soils of the Mangatangi restricting percolation and promoting near-surface runoff, while the deep, porous pumice in the Tahunaatara is less conducive to near-surface runoff, but likely to provide considerable groundwater storage. The hydrology of the loamy Puniu catchment appears to be somewhere in between, with shallow fast groundwater accounting for the majority (32-71%) of the discharge (compared with 6-43% for the other two catchments).

Annual average nitrate yield was predicted to be 3.9-5.1 kg-N ha^{-1} y^{-1} at Tahunaatara, 7.5-10.1 kg-N ha^{-1} y^{-1} at Puniu, and 2.1-3.0 kg-N ha^{-1} y^{-1} at Mangatangi. The third row of Fig. 3 shows the predicted contributions to this nitrate yield from each of the three flow paths (% of kg-N ha^{-1} y^{-1}). Since the concentrations were similar across these catchments, the nitrate yields have a similar pattern to the water flow contributions. As expected, shallow fast groundwater carries the bulk (31-97%) of the nitrate to the stream in all three catchments due to the combination of relatively high concentrations and high water flux. The importance of near-surface flow to nitrate discharge in the Mangatangi catchment (24-63%), however, was not expected. It appears that the hilly contour and clayey soils in this catchment encourage surface runoff and/or shallow subsurface lateral flows, e.g., through artificial drainage systems. These results may indicate an opportunity to reduce nitrate runoff in this catchment using near-surface mitigation options such as riparian strips, constructed wetlands, controlled drainage or permeable reactive barriers. Similarly, the importance of slow groundwater to nitrate discharge in the Tahunaatara catchment (18-63%) was also not expected. Deeper slow groundwater often has extremely low concentrations of nitrate in the Waikato, but in this catchment, the low nitrate concentration (0.2-0.4 mg-N L^{-1}) combined with the large water flux through this flow path (49-81%) resulted in a relatively large annual flux of nitrate. This reflects the presence of a large store of nitrate bearing water in this catchment (although the StreamGEM approach cannot directly estimate storage or transit time). Benefits from land use change or other nitrate mitigation strategies applied in this catchment may therefore not be realised within a short time frame. On the other hand, nitrate yield from slow groundwater appears to be relatively unimportant in the other two catchments (0-15%), indicating a greater potential for mitigation measures to achieve a rapid reduction of nitrate discharges.

The uncertainty attached to these predictions reflects the limited information content of the data, as well as measurement error and model structure error. Using longer or higher-resolution time series may reduce this uncertainty, but only if new information is being added. Including additional *kinds* of data (e.g., groundwater levels, subsurface water chemistry, more representative rainfall and PET data, catchment soil water holding capacity, spatial geology or land use, stream routing) or improving the model structure have greater potential to reduce uncertainty. However, this requires a more complex model, with more parameters that may not be able to be estimated. The relatively simple approach used here, therefore, may be a parsimonious compromise.

Conclusion

Bayesian calibration of a lumped catchment model to widely available monthly water quality data allowed us to quantify the importance of different flow paths (near-surface, shallow fast groundwater, and deeper slow groundwater) to water and nitrate discharges in each catchment. These predictions give us insight into the likely timeframes of nutrient delivery in each catchment, and the likely suitability of alternative mitigation options. The Bayesian approach provides model predictions with uncertainty bounds that reflect the information content of the data and the model. Standard approaches that report only a single "best fit" result may lead to management decisions that are not robust.

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