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RESEARCH ARTICLE

Development of a national-scale framework to characterise transfers of N, P and *Escherichia coli* from land to water

M. S. Srinivasan [a], Richard W. Muirhead [b], Shailesh K. Singh [c], Ross M. Monaghan [b], Roland Stenger [d], Murray E. Close [e], Andrew Manderson [f], John J. Drewry [f], Leo Christopher Smith[g], Diana Selbie [h] and Roger Hodson [i]

[a]Hydrological Processes, National Institute of Water and Atmospheric Research Limited, Christchurch, New Zealand; [b]Farm Systems & Environment, AgResearch Limited, Invermay, New Zealand; [c]Hydrological Modelling, National Institute of Water and Atmospheric Research Limited, Christchurch, New Zealand; [d]Lincoln Agritech Limited, Hamilton, New Zealand; [e]Groundwater Group, Institute of Environmental Science and Research Limited, Christchurch, New Zealand; [f]Soils and Landscapes, Manaaki Whenua Landcare Research Limited, Palmerston North, New Zealand; [g]Farm Systems & Environment, AgResearch Limited, Woodlands, New Zealand; [h]Farm Systems & Environment, AgResearch Limited, Lincoln, New Zealand; [i]Rivers & Streams, Environment Southland, Invercargill, New Zealand

ABSTRACT
A hydrological framework encompassing nitrogen (N), phosphorus (P) and microbial (*E. coli*) transfer from land to water was developed to provide a consistent and rapid approach for assessing the potential impacts of land activity on water quality in New Zealand. A flow partition approach was used to route precipitation via surface and subsurface pathways from land to water. The framework included a typology-based inventory that estimates annual yields of transportable N and P from land, a regional-scale spatial layer that attenuates N in groundwater, and literature-based estimates of *E. coli* concentrations in surface runoff and artificial drainage. Application of the framework in four catchments highlighted the importance of local catchment knowledge of dominant hydrological processes that was needed to ensure flow partitions derived were a realistic representation of transport processes. While the approach was promising, additional refinements are needed to improve process representation (e.g. effects of groundwater lags) and ensure input data (e.g. soil attributes) have appropriate resolution to describe hydrological pathways. We contend that such a framework would provide a consistent and relatively rapid approach for identifying contaminant transfer pathways from land to water that can inform assessments of the potential consequences of land use change and intensification.

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Flow pathways; nutrient transport; hydrology framework; screening tool; flow partition

Introduction

Understanding and identifying transport pathways and the hydrological and biogeochemical processes that control nutrient (nitrogen, N and phosphorus, P) and faecal

CONTACT M.S. Srinivasan ms.srinivasan@niwa.co.nz
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contaminant inputs from agricultural catchments to waterbodies are important steps in the development of effective environmental management strategies. Improved understanding of these pathways and processes is needed to guide freshwater policy responses that continue to be developed as communities seek improved water quality and quantity outcomes. The most recent example for such a response in New Zealand (NZ) is the new requirements proposed by the Ministry for the Environment that are intended to both quickly stop water quality deterioration and set a path to healthier freshwater in a generation. These would require land users to understand and manage environmental risks and adhere to new standards and limits on some farming activities in some regions and catchments (Ministry for the Environment 2019). Similar initiatives have been proposed and implemented in many parts of the world where communities have, or trying to, find an appropriate balance between land use activity and acceptable standards for water quality (e.g. US EPA 2009; Hering et al. 2010). Achieving these goals requires that policy is, ideally, guided by a clear understanding of where contaminant sources originate within catchments, how they are transported to receiving waters, whether they are attenuated along the transport pathway(s) and how management interventions that target either sources or transfer pathways can reduce loads delivered to sensitive receiving environments. These connections between contaminant sources and receiving environments are complex and spatially variable, thus requiring an integrated understanding in space and time of key sources, and hydrological and biogeochemical processes.

There are several ways to quantify the contributions of different pathways for water and contaminant inputs to streams. Direct measurements of contributions from different flow pathways are impractical and resource-intensive, but indirect methods can be employed (Singh and Stenger 2018). While many methods have been developed to elucidate pathway contributions occurring at a storm event scale (e.g. Hooper et al. 1990), others aim to capture longer-term pathway contributions (e.g. Moatar et al. 2017; Woodward et al. 2017; Woodward and Stenger 2018). Combining an understanding of contaminant transport and transformation with hydrological processes and land use enables a prediction of the magnitude, form and timing of contaminants transferred from land to surface water bodies (Croke and Jakeman 2001; Drewry et al. 2006). As has been summarised by Singh and Stenger (2018), gaining a spatially-explicit understanding would have multiple benefits. Firstly, policies and regulations could become more effective and cognisant of the time lag between their implementation and detectable evidence for the desired effect in receiving waterbodies. Secondly, mitigation measures could be located within a catchment to maximise their effectiveness (Wilcock et al. 2013). Thirdly, land use and intensity patterns could be modified to best utilise the spatial variation in natural resources, including soils, and their natural attenuation capacities (Arheimer et al. 2012; Castillo et al. 2014; Hashemi and Olesen 2015).

In 2016, the New Zealand government launched a national-scale land and water management programme, Our Land and Water (OLW) National Science Challenge, to improve the understanding of land management practices and their impacts on water quality. One of the aims of the programme was to develop a framework that can be applied nationally, bringing hydrology and contaminant source, transport and (biogeochemical) transformation processes together. Comprehensive catchment-scale models already provide considerable explanatory power in differentiating the effects of varying land use scenarios (Jayakrishnan et al. 2005; Elliott et al. 2016; Mockler et al.

2016). However, such models seldom consider the key contaminants of concern (N, P and *E. coli*) for water quality in NZ together, or provide a limited representation of the key pathways that are known to be important in their transport and potential attenuation. In addition, it is prohibitively resource-intensive to apply models for each contaminant individually across all NZ catchments. Many of these models require high resolution, catchment-specific input data and specialised science expertise to parameterise, calibrate and validate (e.g. Soil and Water Assessment Tool, Arnold et al. 1998; Hydrologic Simulation Program FORTRAN, Donigian et al. 1984). The conceptual framework proposed within OLW was envisaged as a screening tool, relying exclusively on nationally available databases of soils, geology, climate and river networks, enabling catchments all over NZ to be coherently assessed and categorised based on their likely impact on water quality.

Statistical correlative models such as the Global NEWS model (Seitzinger et al. 2010) have been used in understanding and managing nutrient transport at catchment scale. However, owing to their lack of physical basis, the performance of such correlative models could not be fully tested at diverse spatial and temporal scales (Greene et al. 2015). Spatially-explicit frameworks operating at large timescales, simulating catchment behaviour using national scale databases and readily available (physical) properties of landscape have been reported in the literature (e.g. Leip et al. 2011; Greene et al. 2015). These frameworks, used as screening or assessment tools, generally focus on one or two key contaminants. For example, the Export Coefficient model simulates total N and total P loads from diffused sources for the whole of United Kingdom (Greene et al. 2015); the Unified EMEP model developed in Norway, estimates atmospheric transport and deposition of N across the Europe (Leip et al. 2011); the P index developed in the United States, links sources of P on land and surface transport pathways to water to generate a ranking of a landscape's propensity to lose P (Lemuyon and Gilbert 1993; USDA-NRCS 2011); and the Catchment Land Use for Environmental Sustainability model (CLUES; Elliott et al. 2016), a scenario based model developed for national scale application in NZ catchments, simulates annual N, P, sediment and *E. coli* loadings to water bodies but does not explicitly include hydrological pathways through which these contaminants are transferred from land to water. Other examples include assessments of microbial by-pass flow through soil (McLeod et al. 2008), microbial loss risk at farm and catchment scales (e.g. Oliver et al. 2010; Muirhead 2015; Porter et al. 2017), and P losses at landscape and catchment scales (Heathwaite et al. 2003; Matias and Johnes 2012). However, there are few overarching frameworks that attempt to combine key agricultural contaminants and describe their transport in flow pathways at catchment scale.

In this paper, we describe the development of a nationally-applicable framework and its application to four catchments, considering three key agricultural contaminants – N, P and microbes (*E. coli*). The approach combines a typology-based inventory of contaminant sources with a hydrological framework that routes along potentially five pathways from land to water. Sediment was excluded as the framework is based on catchment-scale hydrological flow pathways which do not consider the dominant erosion processes in NZ catchments as described by Basher (2013). The four case study catchments vary in climate, hydrology, soils, availability of verification and validation data and expert knowledge on hydrological pathways and contaminant transport processes. The specific objectives were to:

1. describe the development of a framework that includes key hydrological pathways linking land to freshwater bodies;
2. combine these pathways with pre-existing contaminant generation and attenuation tools and maps; and
3. assess the performance of the framework for representing contaminant transport within four hydrologically diverse catchments across NZ.

Methods & materials

Description of flow partition approach

In this study, a flow partition approach was used to define the hydrological pathways of water and contaminant transfers. This initially partitioned effective precipitation (=precipitation – evaporation; hereafter referred to as 'precipitation') into four potential hydrological pathways: surface runoff (SF), interflow (IF), shallow (local) groundwater flow (SGF) and deep (regional) groundwater flow (DGF). The total flow at a catchment outlet was simulated as the summation of flows from all pathways. The estimated contaminant source loads were split across these pathways according to flow through each one of them. In two case study catchments, an additional artificial drainage pathway (sub-surface) was considered. Sequentially, artificial drainage followed interflow, which then preceded shallow groundwater flow. The partition approach was based on information sets and layers that included land use, soil type, topography, thickness of soil layers, predicted distribution of artificial drainage structures, precipitation, air temperature, geology and an expert knowledge of the case study catchments.

When calibrating a model using observed flow at a catchment outlet, the predicted flow can be arrived at using several possible combinations of surface and sub-surface flow pathways. This problem, termed as 'equifinality', has been identified as a major source of error in model simulation, specifically when models are calibrated to represent internal catchment hydrological behaviour using only flows measured at catchment outlets (Beven 1993; Beven and Freer 2001). In addition to catchment physical and hydrological data layers, expert knowledge (from co-authors of this paper) and information from previous studies either in those catchments or from neighbouring similar catchments, where available, was used to guide the calibration process that reduced the error and uncertainty caused by equifinality.

A semi-distributed catchment model, Hydrological Predictions for the Environment (HYPE) (Lindström et al. 2010) was used to partition precipitation into four flow pathways described above. For the model application, the surface drainage catchment was divided into first order sub-catchments. No groundwater boundaries were considered as those data were not available nationally. At the outlet of each sub-catchment, all flow pathways converged to generate a combined streamflow, which then was routed through a surface stream network to the catchment outlet. No abstraction of flow from the river network (e.g. for irrigation), managed storage and release within the network (e.g. for hydropower generation) or in-stream attenuation of contaminants was considered as such data are seldom available at a national scale. Each sub-catchment included a range of soils and land use derived from nationally-available spatial data layers. The digital river network developed by Snelder and Biggs (2002), and a 30-m digital elevation model and land cover databases developed by Newsome et al. (2008, 2013) were used to derive the flow and physical networks for the catchments. Soil data were derived from a digital soil map database, S-Map (https://smap.landcareresearch.co.nz/). Regional scale geology data were derived from QMAP (Rattenbury and Heron 1997).

Conceptually, the HYPE model does not consider soil horizons but divides the subsurface environment (referred to as 'soil' hereafter) into three layers – the top layer, or soil layer 1, is associated with surface runoff. The layer below (soil layer 2) is associated with interflow, artificial drainage and shallow groundwater flow. The bottom or soil layer 3 is associated with deep groundwater flow. The shallow groundwater corresponds to local, unconfined aquifer and the deep groundwater represents regional scale systems. Each layer has corresponding storage; water in excess of storage is routed either to the layer below or through a flow pathway. The storage information could be derived either from soil (for the top 1.5 m), geology database, or through calibration. The HYPE model allows inclusion of groundwater aquifer information if available, but that option was not chosen in the study, as those data were not available nationally.

Artificial drainage such as mole-tile pipe drainage is prevalent in two of the case study catchments, Aparima and Oreti. However, no maps on the distribution and location of drains were available. Pearson (2015) developed a procedure based on soil permeability and drainage class for predicting catchments with artificial drains in the region where Aparima and Oreti catchments are located; this procedure was therefore adopted for this study. The HYPE model is not sensitive to the actual location of sub-surface drains within the catchment but to their drainage density, as that influences the rates and volumes of flows transported. The amount of flow via artificial drainage was a direct function of water head above the drainage structure.

Daily stream flow measured at the catchment outlet and 5-km grid interval precipitation, relative humidity, solar radiation and temperature data for the period 2000–2016 were obtained from a publicly-available databases (CliFlo 2018; NIWA 2018). During the calibration process, the model parameters were varied depending on catchment hydrological conditions (stormflow or baseflow) until the magnitude and timing of the simulated flows matched the observed. Based on previously published studies on the HYPE model (e.g. Lindström et al. 2010) and the specific objective of this study (flow partition through matching of simulated and observed flows), a selection of model parameters was adjusted during the calibration process. The parameters adjusted during the model calibration process are listed in Table 1, along with their links to specific flow pathways. Initial parameter values and their range were estimated from literature (e.g. Pierong and Takman 2014; Hundecha et al. 2016). Nationally-derived information such as baseflow index (Singh et al. 2018) and potential groundwater recharge (Singh et al. 2019) were also used in parameterising the model.

In addition to observed flow data, the calibration process was also guided by co-authors' expert knowledge of the catchments as well as information from previously published studies (e.g. Monaghan et al. 2016; Woodward and Stenger 2018). For example, for poorly draining soils on relatively flat topography, such as those characterised in the Oreti and Aparima catchments, surface and shallow sub-surface processes

Table 1. Parameters altered during the calibration of the HYPE model to apportion pathway flows.

Process/store	Parameter description	Hydrological flow and processes most influenced
Water holding capacity	Fraction of soil water available for potential evapotranspiration	Surface runoff
	Wilting point as fraction of soil depth	Surface runoff
	Effective porosity as fraction of soil depth	Surface runoff
Percolation	Maximum percolation capacity	Interflow, shallow groundwater flow
Surface runoff recession	Soil recession coefficient	Surface runoff
Surface runoff	Threshold for macro pore flow	Surface runoff, interflow, shallow groundwater flow
	Threshold soil water content as a fraction of soil depth for macro pore flow and surface runoff	Surface runoff, interflow, shallow groundwater flow
	Fraction of macro pore flow	Surface runoff, interflow, shallow groundwater flow
	Fraction of surface runoff	Surface runoff
	Recession coefficient for surface runoff	Surface runoff
Evapotranspiration	Threshold soil water for activation of potential evapotranspiration	Water balance
	Temperature correction for elevation in relation to mean sub-catchment elevation	Water balance
Precipitation threshold	Threshold elevation for precipitation adjustment	Water balance
Groundwater recession	Recession coefficient for ground water	Shallow and deep groundwater

dominate flows. Conversely, the Waiotapu catchment was assumed to be dominated by (deep) groundwater flows, as indicated by the very stable stream flow hydrograph and chemistry-assisted hydrograph separation (Woodward and Stenger 2018), the relatively high mean residence times determined on baseflow samples (unpublished data), and groundwater modelling (Sarris et al. 2019a). In the Oreti catchment, observations from a plot scale tile-drain study (Monaghan et al. 2016) guided the calibration process. No such specific expert knowledge on catchment hydrology was readily available for the Waitangi catchment and thus the calibration process was guided only by flows measured at the catchment outlet.

The HYPE model was run at a daily time step, and the match between daily simulated and observed flows were evaluated using the Nash-Sutcliffe efficiency metric (NSE; Nash and Sutcliffe 1970). Model calibrations were balanced between maintaining the dominant pathway as guided by expert knowledge and previous studies, and the best match between observed and simulated flows as evaluated using the NSE metric. Once the model was calibrated for each case study catchment, the flow transferred along each pathway was calculated as a proportion of total daily flow simulated at the catchment outlet. These daily flow partitions were averaged to provide an annual value for each pathway for every year of simulation. Annual flow partition values from 2001 to 2016 were used for calculating N, P and *E. coli* transport. This approach constituted the framework discussed throughout this paper. A schematic representation of the framework is shown in Figure 1. The generated contaminant yield estimations and their transport along surface and sub-surface pathways are described in subsequent sections.

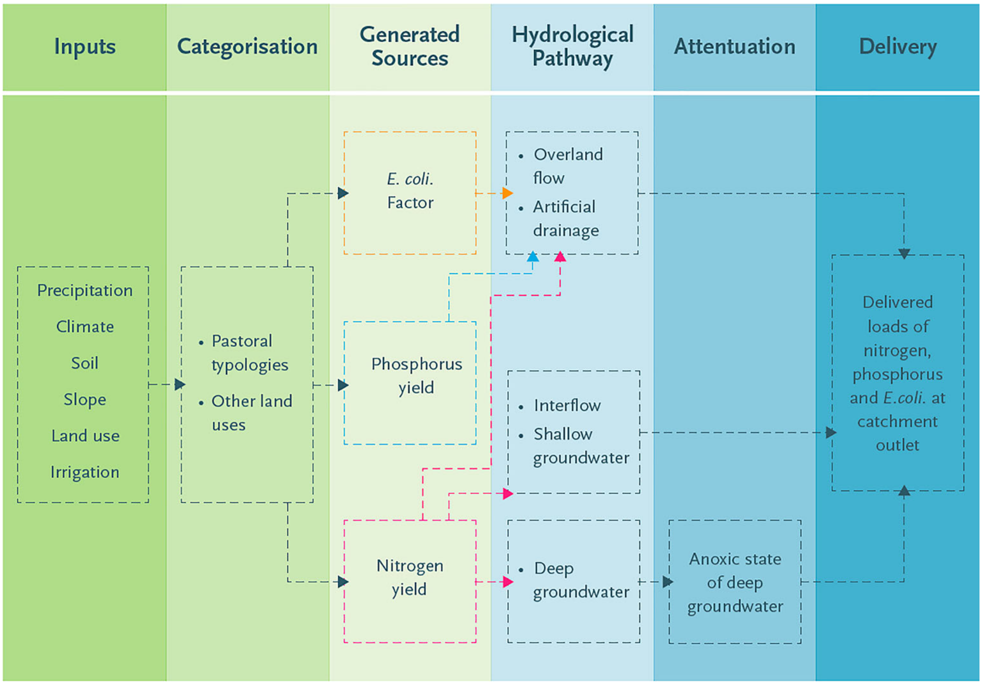

Figure 1. A schematic representation of the framework used to characterise transfers of N, P and *E. coli* from land to water.

Description of case study catchments used for framework validation

To test the utility of the framework, it was applied in four case study catchments across a range of climatic and hydrological regions present in NZ. Climatically, the Waitangi catchment (see Figure 2) is located within a warm, sub-humid zone while the Waiotapu, Aparima and Oreti catchments lie within cooler, temperate zones (NIWA 2018). The Oreti and Aparima are dominated by poorly draining soils that are artificially drained (Monaghan et al. 2016), while the Waiotapu catchment is dominated by deep groundwater

Table 2. Physical, climatic and hydrological description of the case study catchments where the framework was applied.

	Waitangi	Waiotapu	Aparima	Oreti
Surface drainage area (km^2)	302	308	1,191	3,304
Outlet location (NZTM)	1695269E 6095808N	1891505E 5740654N	1221285E 4862374N	1235612E 4858800N
Elevation range (m above mean sea level)	7–384	292–965	1–1,559	3–1,985
Geology*	HS, VA	VA	HS, AI, SS, VB	HS, SS, AI
Annual precipitation (mm)	1,864	1,389	1,160	1,205
Mean flow based on measurements (m^{3}s^{-1})	8.0	2.8	33.3	89.2
Drainage density (mkm^{-2})	1,615	1,537	1,698	1,592
Dominant land use(s)**	P	P, EF	P, T, IF, EF	P, T, IF, EF

*HS: Hard Sedimentary rocks, VA: Volcanic Acidic, SS: Soft Sedimentary, AI: Alluvium, VB: Volcanic Basic
**P: Pastoral, EF: Exotic Forestry; T: Scrub, Tussock; IF: Indigenous Forest.

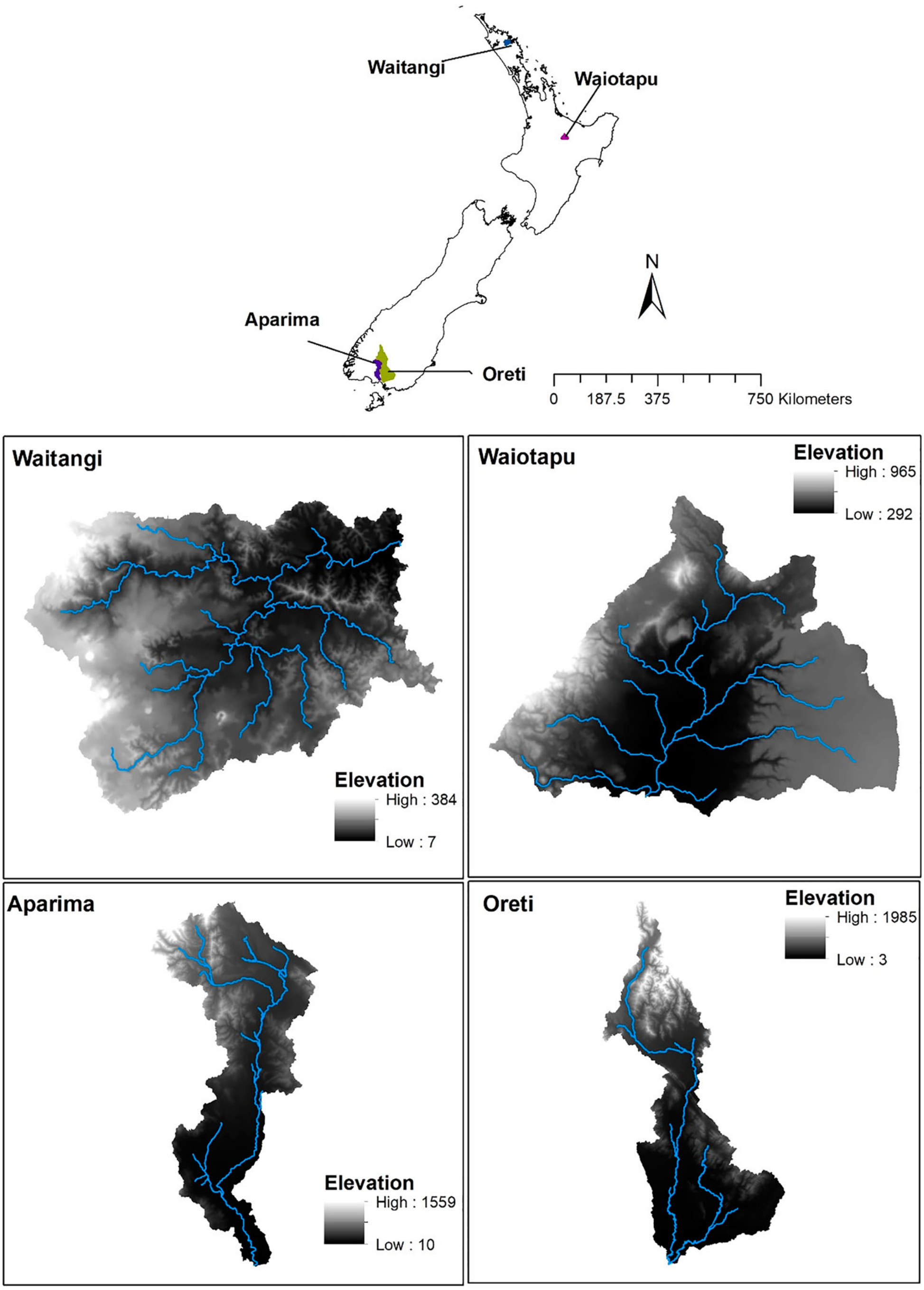

Figure 2. Geographical location of the case study catchments. Catchment boundary, flow network and elevation are shown. Elevation in metres above mean sea level.

flows (Woodward and Stenger 2018). A brief description of known catchment characteristics is presented in Table 2.

Inclusion of contaminant inventory tools, attenuation maps and literature-based estimates to the framework

Generation and transport of N & P

A typology-based approach was used to derive N and P yields from pastoral and non-pastoral farms across NZ. Dairy farm typology categories were based on climate (rainfall and winter soil temperature), landscape (slope) and soil attributes (such as drainage class) that are known to influence N and P loses from land to water and are described in detail in Monaghan et al. (2018). These factors were combined with land use (e.g. dairy, sheep & beef, forestry and others) information to derive estimates of annual transfers (kg ha^{-1}) of N and P to water. Table 3 lists annual yields of N and P from pastoral and non-pastoral farms, based on Monaghan et al. (2018), used in the framework. For dairy land use, N and P losses generated (and thus available for transport) were estimated using the Overseer Nutrient Budgets® tool (henceforth *Overseer*, https://www.overseer.org.nz/) using information derived from DairyBase records. DairyBase is a nationally available database maintained by the dairy industry body, Dairy New Zealand, and includes physical and financial information on a selection of dairy farms across NZ.

For sheep and beef farms, typology categories focussed on the productive potential of the farmed landscapes (mainly governed by slope, temperature and rainfall factors) as a primary consideration, in recognition of the driving influence that production potential exerts on farm N loss risk from non-dairy land in particular. Due to the availability of limited data, sheep and beef farm typologies were based on prior-established farm classes used in the Beef+Lamb New Zealand Economic Service Sheep and Beef Farm Survey (BLNZ 2018). This is a national-level annual survey involving a sample of approximately 500 sheep and beef farmers and uses eight farm classes and six production regions to represent a total of 17 sheep and beef farming combinations across NZ. Nutrient budgets for each of these farm classes were constructed in *Overseer* and parameterised as described in Monaghan et al. (in preparation). For land uses not described above, N and P generated yield data were determined from a literature search of NZ-based studies, including measured and modelled data, with an emphasis on the peer-reviewed literature (Drewry 2018). The yields of N and P generated from land use activity were assumed to represent total forms of both nutrients; in the case of N, the predominant proportion of this was assumed to be nitrate-N.

In the case of N transfers, we made the simple assumption that pathway apportionment was based on the proportional flow computed by HYPE. Thus, for the example of a sub-farm polygon (derived from the intersection of the farm typology N loss layer and the flow partition layer) losing 40 kg N ha^{-1} y^{-1} and where DGF represented 30% of flow, N yield to the DGF flow pathway equalled 40 * 0.3 = 12 kg N ha^{-1} y^{-1}. This N calculation step was applied to all five of the potential flow pathways that might be active at any given location. Attenuation was assumed to occur for N transported via SGF and DGF pathways and is described in more detail in a later section.

Transfers of P to water from each farm typology unit were assumed to occur via surface and artificial drainage pathways only. Preliminary analyses indicated there were relatively small amounts of artificial drainage flows from unrealistically large proportions of the Aparima and Oreti catchment areas, possibly due to poor spatial representation of artificial drainage within the HYPE model. To overcome this spatial artefact, we therefore

Table 3. Inventory of modelled and assumed yields of N and P for pastoral farm typologies and other categories of land use or cover. Values are assumed to represent N and P losses in combined drainage and surface runoff flows, although it should be recognised that studies (measured and modelled) did not always measure or model secondary pathways of loss; further details can be found in Monaghan et al. (in preparation) and Drewry (2018).

Land use	Slope	Moisture	N loss (kg N ha^{-1} y^{-1})		P loss (kg P ha^{-1} y^{-1})	
			Median	Range*	Median	Range*
Dairy	Flat	Dry	29.5	23–38	0.85	0.6–1.2
		Moist	39	29–45	1.05	0.6–1.4
		Wet	48.5	34–55	1.25	0.6–1.4
		Irrigated	55.5	33–82	0.95	0.8–1.1
	Rolling	Dry	27	22–36	1.0	0.9–1.6
		Moist	32	25–44	1.5	0.9–1.9
		Wet	45	28–53	1.8	0.9–1.9
		Irrigated	52	29–63	1.3	1.1–1.6
	Easy Hill	Dry	28	26–36	1.0	0.9–1.6
		Moist	32	25–44	1.5	0.9–1.9
		Wet	45	28–53	1.8	0.9–1.9
		Irrigated	52	29–63	1.3	1.1–1.6
Sheep / Sheep & Beef	Flat	Dry	7		0.4	
		Moist	18	15–21	0.6	
		Wet	24	18–30	0.75	0.7–0.8
		Irrigated	20	17–23	0.6	
	Rolling	Dry	7.5	7–8	0.35	0.3–0.4
		Moist	11.5	9–14	0.7	
		Wet	17.5	11–24	0.8	
		Irrigated	11.5	9–14	0.7	
	Easy Hill	Dry	5	4–6	0.5	
		Moist	8.5	8–9	1.0	
		Wet	9	7–11	1.6	
	Steep	Dry	4.5	4–5	0.6	
		Moist	6	4–8	1.6	
		Wet	6.5	5–8	2.8	
Beef	Flat	Dry	13		0.6	
		Moist	32	27–37	0.7	
		Wet	38	32–44	1.15	1.0–1.3
		Irrigated	34.5	29–40	0.8	
	Rolling	Dry	13	12–14	0.5	
		Moist	20.5	15–26	0.9	
		Wet	27	20–34	1.2	
		Irrigated	20.5	15–26	1.2	
	Easy Hill	Dry	9	7–11	0.7	
		Moist	15.5	14–17	1.5	
		Wet	15.5	12–19	2.4	
	Steep	Dry	8	6–10	1.0	
		Moist	10.5	8–13	2.4	
		Wet	12	10–14	4.3	
Deer	All	Dry	7	7–9	0.75	0.2–1.0
		Moist	12	9–12	1.9	0.4–2.8
		Wet	18		0.8	0.6–1.0
Other pastoral support land used for winter forage crop grazing	Flat	Dry	17	17–18	0.35	0.3–0.4
		Moist	41	32–41	0.65	0.5–0.8
		Wet	49	39–49	1.0	0.8–2.0
		Irrigated	36	31–45	0.7	0.6–0.8
	Rolling	Dry	17	17–19	0.4	0.3–0.4
		Moist	33	25–36	0.8	0.7–0.8
		Wet	45	33–45	1.4	0.8–2.1
		Irrigated	35	31–36	0.8	0.7–1.0
Arable and mixed Crops	Flat	All	13.5	1–113	0.1	0.1–2.9
Vegetable growing	Flat	All	72	2–220	1.9	
Viticulture	Flat	Unknown	10	1–37	0.2	0.1–0.5

(*Continued*)

Table 3. Continued.

Land use	Slope	Moisture	N loss (kg N ha^{-1} y^{-1})		P loss (kg P ha^{-1} y^{-1})	
			Median	Range*	Median	Range*
Forestry	All	All	4	1–28	0.4	0.1–1.3
Native Bush	All	All	2	1–7.1	0.3	0.1–0.6

*Ranges reflect variation caused by contrasting soil drainage and temperature typology attributes.

assumed that P transfers via artificial drainage only occurred for locations where artificial drainage flow exceeded a threshold of 0.3 (30%) of rainfall surplus. Artificial drainage pathway P yields for these locations were then calculated as the lesser of [sub-farm typology P yield per hectare] or [0.3 kg P per ha]; this latter figure is assumed to represent a typical artificial drainage P yield as documented in studies by Monaghan et al. (2016) and other unpublished reports. Transfers of P via the SF pathway were then calculated as the difference between total (sub-farm polygon) P yield and artificial drainage P yield.

E. coli *generation and transport tool*

E. coli generation and transfer was only considered from pastoral land use and *E. coli* from other land uses was assumed to be zero. Among the pathways, *E. coli* transport in surface and artificial drainage flows were considered and *E. coli* concentrations of 2×10^8 and 4.8×10^7 cfu m^{-3}, respectively, were assumed after Dymond et al. (2016) and Monaghan et al. (2016). Estimates of flow derived from the HYPE model were then combined with these mean concentrations to determine annual loads of *E. coli* generated per ha for the pastoral land use area. These annual loads of *E. coli* were compared to other published studies and the spatial distributions investigated.

N attenuation spatial layer

Since N attenuation during transport via groundwater influences the amount of N delivered to water bodies in many NZ catchments (e.g. Collins et al. 2017; Rivas et al. 2017), a pre-existing N-attenuation layer developed by Close et al. (2016) was included in the framework. This layer was available for Aparima, Oreti and Waiotapu catchments only. Based on Close et al. (2016), the spatial layers of predicted redox status for the Southland (Aparima and Oreti) and Waiotapu catchments were developed by Wilson et al. (2018) and Sarris et al. (2019a). The above-mentioned studies applied a linear discriminant analysis (LDA, from Close et al. 2016) on measured groundwater N data and linked this to spatial data layers such as geology, land use, topography and soil properties to discriminate between the groundwater redox states. More details on LDA can be found in Tabachnick and Fidell (2013).

The amounts of N attenuation for different redox zones have previously been incorporated into groundwater transport modelling studies as calibrated first-order decay rates (Sarris et al. 2019a, 2019b). This approach is unsuited for the simple approach used for describing groundwater processes in the framework presented here. Simple percentage removal estimates for N attenuation were therefore used as follows: reducing zones removed 70% of N transported via SGF and DGF pathways; mixed zones removed 35%; and oxic zones removed 5%. These simple percentage removal estimates were derived from the first-order decay rates obtained from the modelling studies (Sarris et al. 2019a, 2019b) using these redox zones for an arbitrary time period of 1 year. Note that the first-order decay rates for reduced zones from the modelling studies were similar to rates measured in NZ for reduced groundwater systems (Burbery 2018), although these measurements were carried out at a local scale and in only two regions. As these percentage removal estimates have been derived from catchment scale studies, it could be expected that optimisation or calibration of these estimates against observation data at the national scale would improve the performance of the framework model for N in the future. To a limited extent these N removals incorporate N that is likely removed via in-stream processes, such as N uptake by aquatic plants and algae, or denitrification. Only the shallow groundwater redox layer was used, as the framework approach assumed that all groundwater re-enters the surface system at the next downstream node.

Results and discussion

Estimates of total and partitioned flows derived using the HYPE model

Daily observed, simulated and partitioned flows for the Waiotapu and Oreti case study catchments are shown as examples in Figures 3 and 4. For clarity and readability, only data from an average year,defined by annual precipitation, are shown. Statistically, the match between daily observed and simulated flows was best for the Waitangi catchment and poorest for Waiotapu (see NSE metric, Table 4). Based on the calibrated model, the derived daily partitioned flows were aggregated annually. An average of these annual values for each pathway for the simulation period (2001–16) are shown in Table 4 for the four case study catchments.

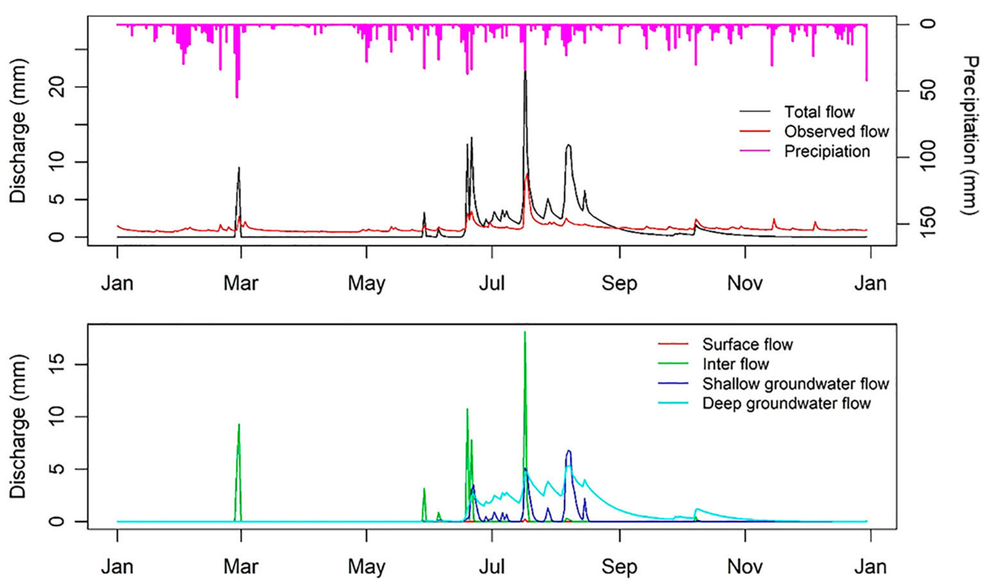

Figure 3. Comparison of daily observed and simulated flows for an average year (2004) and partition of flows via different pathways in the Waiotapu catchment.

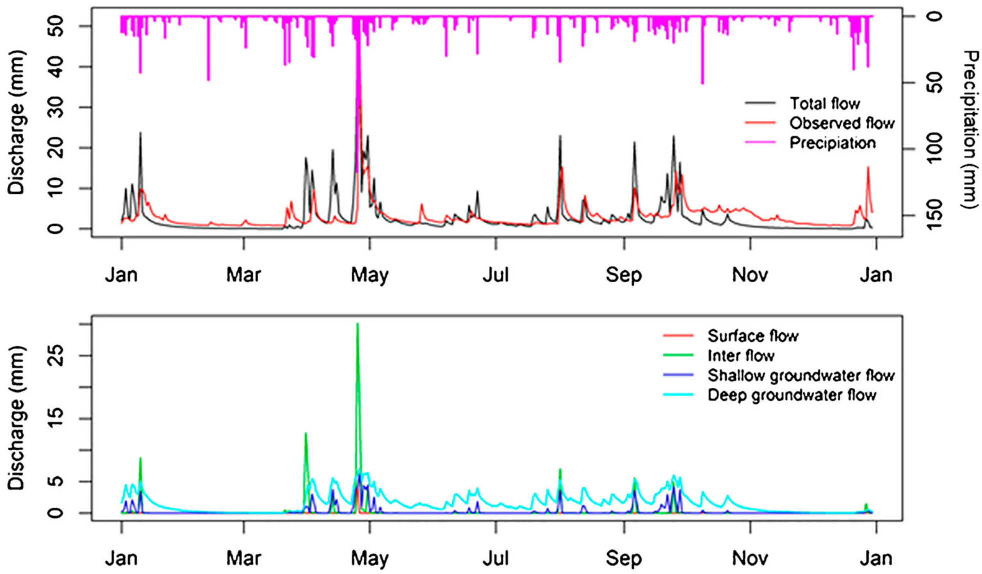

Figure 4. Comparison of daily observed and simulated flows for an average year (2010) and partition of flows via different pathways in the Oreti catchment.

In general, deep groundwater flow contributions dominated the outflow in all catchments. In the Waitangi catchment, where no previous knowledge of hydrological flow pathways was used during calibration, most of the flow (94.4%, see Table 4) was simulated to occur via the deep groundwater pathway. There was no independent source of data to validate this predicted high groundwater contribution. In contrast, deep groundwater flows in the Aparima and Oreti catchments contributed two-thirds of flows simulated at the outlet, with artificial drainage contributing an additional one-sixth. In the Waiotapu catchment, based on expert knowledge and information from an earlier study (Woodward and Stenger 2018), the model calibration was biased towards groundwater pathways (shallow and deep), and these two pathways together contributed 89% of all flows simulated at the outlet. These annual flow proportions were used directly to estimate contaminant transport within each pathway.

The spatial distribution of shallow and deep groundwater pathway contributions (average of annual partition values from 2001 to 2016) for the Waiotapu catchment is

Table 4. Average annual apportionment of flows transferred along surface and sub-surface pathways to the catchment outlet for the case study catchments, based on HYPE model simulations. The Nash-Sutcliffe efficiency metric is indicative of model performance for the simulation period, 2001–16.

	Apportionment of flows along each pathway expressed as a percent of total flow simulated at the catchment outlet					
Catchment	Surface runoff	Interflow	Artificial drainage	Shallow groundwater flow	Deep groundwater flow	Nash-Sutcliffe efficiency
Waitangi	1.6	1.1	No artificial drainage considered	2.9	94.4	0.45
Waiotapu	0.01	10.4	No artificial drainage considered	23.0	66.6	0.20
Aparima	0.4	8.7	16.8	8.8	65.3	0.44
Oreti	0.4	8.6	17.9	9.7	63.4	0.30

shown in Figure 5. Spatial distributions of flow partitions through other pathways, and for other catchments are provided as supplementary material. While the calibration process in the Waiotapu catchment was biased towards a dominant deep groundwater system, the magnitude of deep groundwater contribution across the catchment varied. For instance, the western parts of the catchment characterised by fine textured soils and steep slopes were more conducive to surface runoff and interflow. Groundwater contributions dominated coarse textured and less-steep eastern parts. In the Aparima and Oreti catchments (see Figure 6 for Oreti catchment; only surface runoff and artificial drainage apportionments are shown; for other pathways and catchments, refer to the supplementary material), surface runoff dominated flow contributions in head waters, whilst artificial drainage was more evident on the flatter, lower parts of the catchments. In the Waitangi catchment, where the calibration focussed on matching simulated flows to those observed at the catchment outlet, deep groundwater dominated the flow hydrograph (for flow hydrograph and apportionments for the Waitangi catchment, refer to the supplementary material).

While it is difficult to evaluate the accuracy of flow partitioned through different pathways, such as those presented in Table 4, the partition values were tested for their consistency using two levels of validation data for the case study catchments – qualitative information at catchment scale for the Waiotapu catchment and quantitative information based on a plot-scale study in the Oreti catchment. Woodward and Stenger (2018), who conducted a three-component hydrograph separation in the Waiotapu catchment,

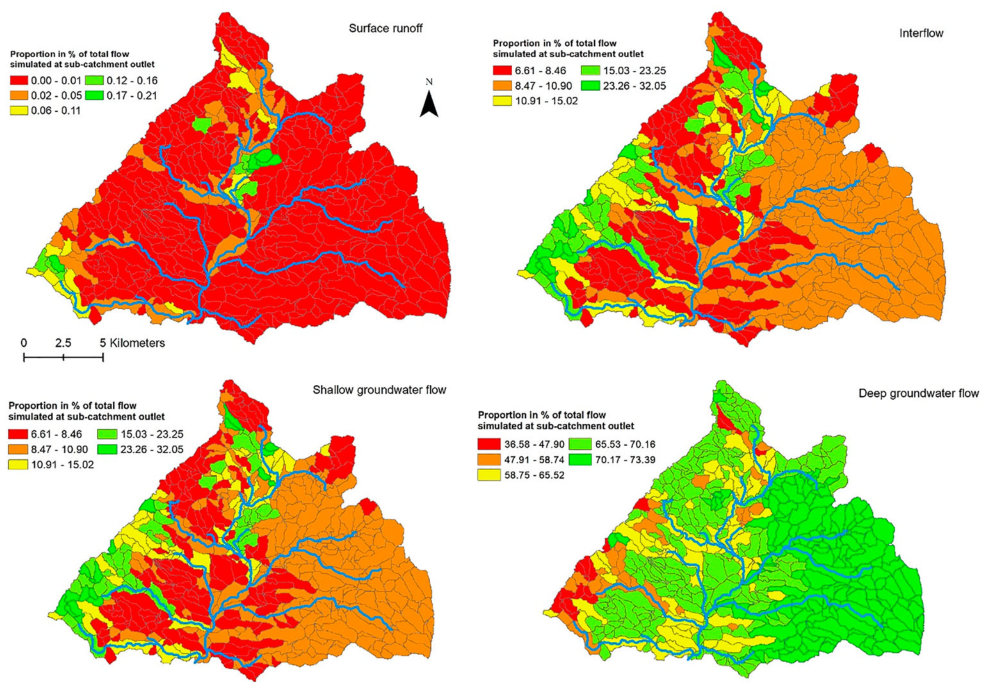

Figure 5. Estimated flow contribution (percentage of total simulated) to the Waiotapu catchment outlet via surface water and groundwater pathways. Blue lines indicate surface drainage network.

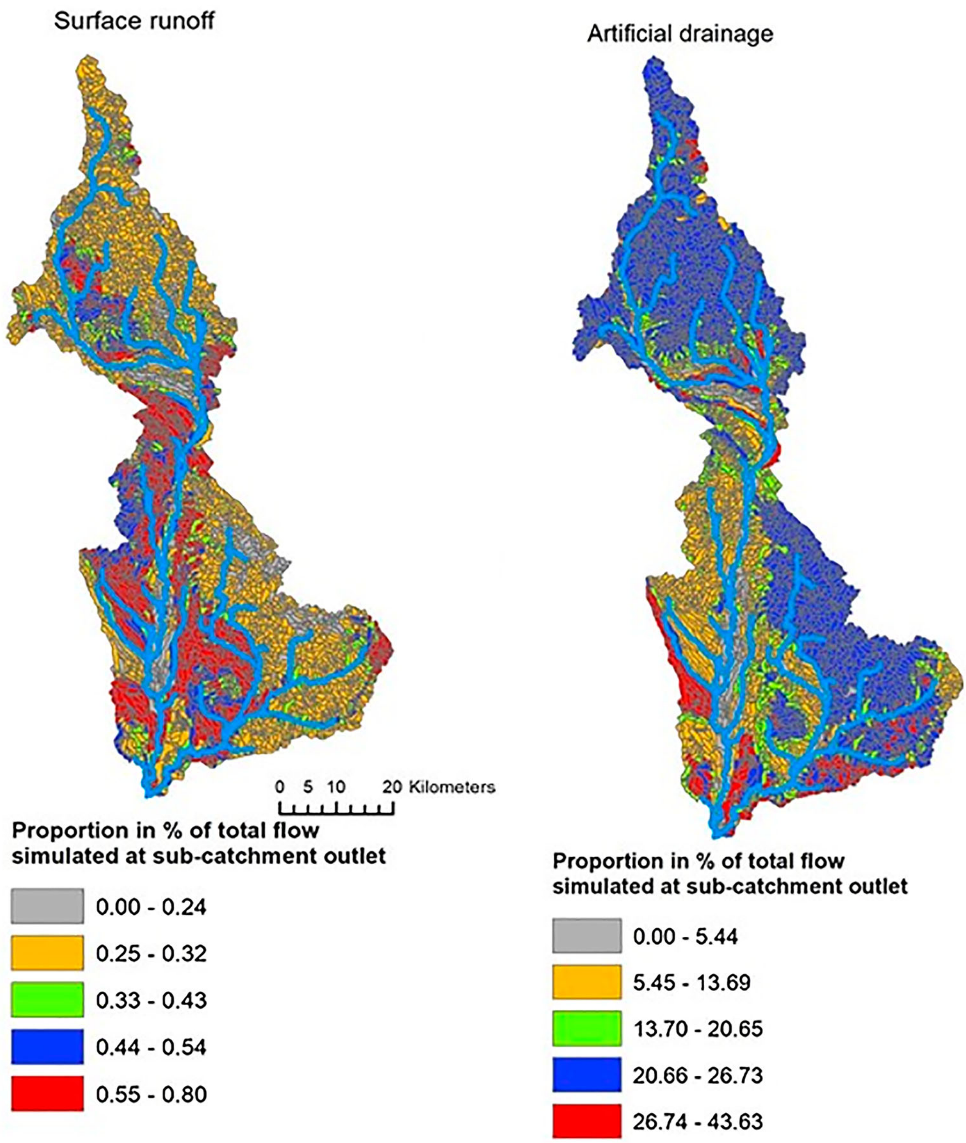

Figure 6. Estimated flow contributions (percentage of total simulated) to the Oreti catchment via surface runoff and artificial drainage. Blue lines indicate surface drainage network. Percent contributions of flows from other pathways are included in the supplementary material.

indicated shallow and deep groundwater flow contributions to be the highest, which is consistent with the modelled flow partitions documented here (23% SGF and 67% DGF modelled). Based on a three-year plot scale study within the Oreti catchment, Monaghan et al. (2016) reported that 62% and 25% of total flow recorded came from artificial drainage and surface runoff pathways, respectively. These plot-scale observations were used during the calibration process although the model-simulated artificial drainage flow and surface runoff never exceeded 44% and 19%, respectively (the latter representing both surface runoff and interflow). Discrepancies between these plot-scale study results and model predictions for this catchment could be attributed to a combination of reasons that include, uncertainty associated with (i) model input information on the extent of artificial drainage (ii) challenges of hydrological connectivity and upscaling of plot-scale study results to catchment scale, as highlighted by Cerdan et al. (2004) and Srinivasan et al. (2007); and (iii) insufficient resolution of national scale datasets on climate, geology and soils for representing hydrological processes at smaller (sub-catchment) scales.

The flow partition approach represents a simplistic method for distributing and routing effective precipitation through various pathways from land to receiving waters. Although it is a relatively unsophisticated approach, consideration of hydrological pathways does provide two distinct advantages over empirical approaches: (1) an ability to separate and represent pathways according to their lag times (e.g. separation of DGF from SF as they link land and water at different time scales); and (2) an ability to include attenuation and mitigation practices that are specific to hydrological pathways (e.g. application of attenuation to groundwater-transported N as described in this study). Flow contributions through various pathways are seldom measured in catchments; hence contributions through various flow pathways could only be estimated based on indirect methods as described in Singh and Stenger (2018). Use of geochemical and isotopic tracers to track the pathways have also been widely reported in the literature (see Inamdar 2011 for a review of the methods available). The simplified approach of differentiating between three conceptual pathways, often labelled near-surface pathway (comprising overland flow, interflow and artificial drainage), shallow (local) groundwater flow, and deep (regional) groundwater flow, has proven useful in previous catchment-scale studies (e.g. Hesser et al. 2010; O'Brien et al. 2013; Woodward et al. 2013).

In catchments where the expert knowledge is weak, the flow partition values can be tested using multi-model and multi-basin approaches. In a multi-model approach, as has been applied by Velázquez et al. (2013) and Srinivasan et al. (2019), models that vary in structure and process representation (conceptual, lumped/distributed, empirical/physically-based and others) can be used to simulate and cross-examine the hydrological behaviours of catchments and consistency of flow pathway attributions. In a multi-basin approach, a given hydrology model is applied simultaneously to a cluster of catchments within the same region and the outputs (such as simulated flows, flow pathway attributions) compared to locate outlier catchments, described as those that do not follow 'population' behaviour. This approach is also referred to as comparative hydrology in the literature (Falkenmark and Chapman 1989; Sivapalan 2009; Blöschl et al. 2013; Donnelly et al. 2014).

Routing N, P and E. coli *through flow pathways*

The relative contributions of water and entrained contaminants through different flow pathways, as defined by the flow partitioning model, for the four catchments are shown in Figure 7. Contrasting patterns of flows and contaminant losses are most evident when the Oreti and Aparima catchments are compared against the Waiotapu and Waitangi catchments. The latter catchments are identified as having predominantly groundwater pathways of flow being active, with very little surface flow predicted. Consequently, a large majority of the N loss from land is deemed to be transported to groundwater and losses of P and *E. coli* are predicted to be accordingly low. This

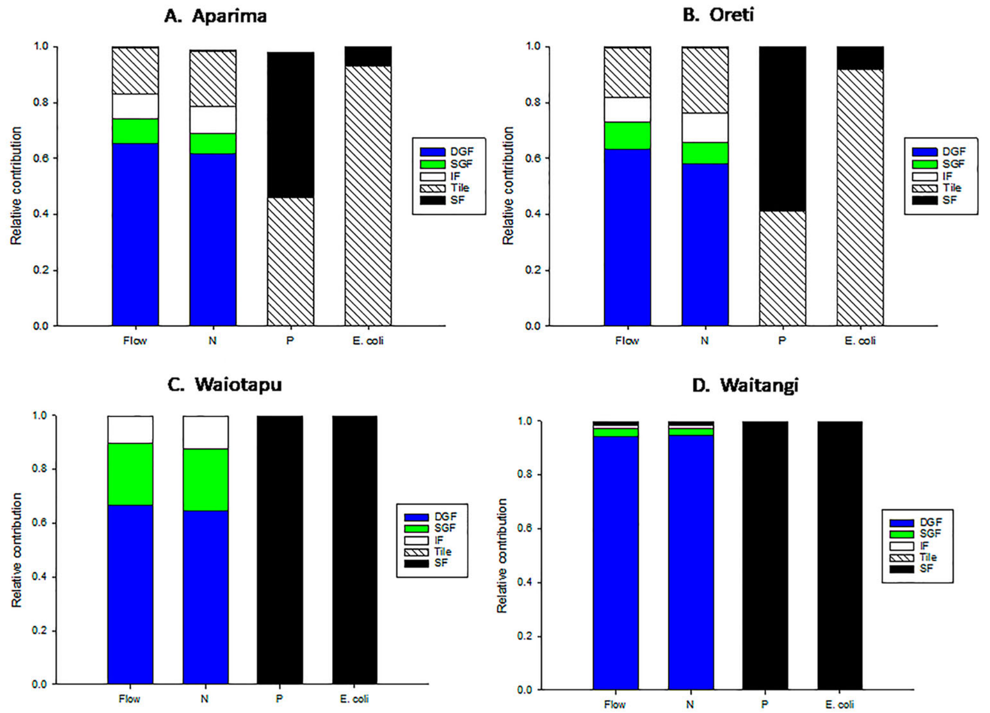

Figure 7. Estimates of relative pathway contributions of N, loads as simulated using average annual flow apportionments, for the case study catchments. SF – Surface runoff; IF – Interflow; Tile – Subsurface artificial drainage; SGF – Shallow Groundwater Flow; DGF – Deep Groundwater Flow.

observation is consistent with the permeable and free-draining nature of the soils and vadose zones within these catchments. In the Waitangi catchment, the absence of an attenuation layer meant that all generated N loads were calculated to be delivered to the catchment outlet.

In contrast, artificial drainage and surface flow pathways were identified as important conduits for water and contaminant transfer in the Aparima and Oreti catchments, where less permeable and poorly-drained soils are more common. Combined artificial drainage and surface flow yields of water and N in these catchments represent *ca* 20% of total flow, with interflow accounting for another 10% of combined flow and N discharge. A consequence of the more active surface and artificial drainage flow pathways is the rapid discharge of P and *E. coli* entrained in these flows (Figure 7). The interquartile range of annual *E. coli* loads transported in artificial drainage in both Southland catchments was estimated to be from 10^{12} to 10^{14} cfu ha^{-1} representing 92% and 82% of total generated loads for the Aparima and Oreti catchments, respectively. The interquartile range of generated *E. coli* loads for the three catchments where the surface flow pathway was active (Aparima, Oreti and Waitangi) was estimated to range from 10^{11} to 10^{13} cfu ha^{-1} y^{-1}. The large *E. coli* yields simulated at Waitangi agrees with observations made by the local regional council (Northland Regional Council 2014). In contrast, the interquartile range of *E. coli* loads in the Waiotapu catchment was substantially lower, ranging from 0 to 10^{9} cfu ha^{-1} y^{-1}. Surface flow was estimated to contribute between 50% and 60%

of the P discharged from land in the Aparima and Oreti catchments, with artificial drainage assumed to account for the remainder of losses.

Consideration of the transport pathway is necessary to calculate N attenuation during transport through groundwater. As noted above, significant proportions of farm N discharges to water in the Aparima and Oreti catchments occurred via surface, interflow and artificial drainage pathways where N attenuation processes can be practically insignificant, thus not considered in the framework. These rapid flows were estimated to convey approximately one-third of the N predicted to eventually enter the main stems of the Aparima and Oreti rivers. Application of the simple N attenuation model (see section 2.3.3) to the remaining N load that was calculated to enter groundwater in the Aparima, Oreti and Waiotapu catchments suggested that between 20% and 25% of the N discharged from land was attenuated. This amounted to 3–4 kg N ha^{-1} y^{-1}.

The ability of the framework approach described here to predict loads of N and P discharged from the Aparima and Oreti catchments was assessed by comparing our estimates of N and P delivery to the river networks with loads measured at catchment outlets, as determined by Environment Southland, the local regulatory authority. These estimated and measured losses were converted to equivalent specific annual yields (kg ha^{-1}) and are presented in Figure 8. Reasonable agreement between estimated and measured losses is evident for N for both catchments, with each measured as discharging about 80% of what the framework estimated to be leaving farms and from gross calculations of groundwater attenuation. This difference should in theory represent N attenuated in surface water and any lag effects due to groundwater transport. However, the estimate for the N yield delivered to the catchment outlet at Waiotapu is approximately twice as high as the N yield calculated from monthly water quality sampling and flow monitoring data (unpublished data). Two factors could explain this discrepancy. Firstly, the extent of

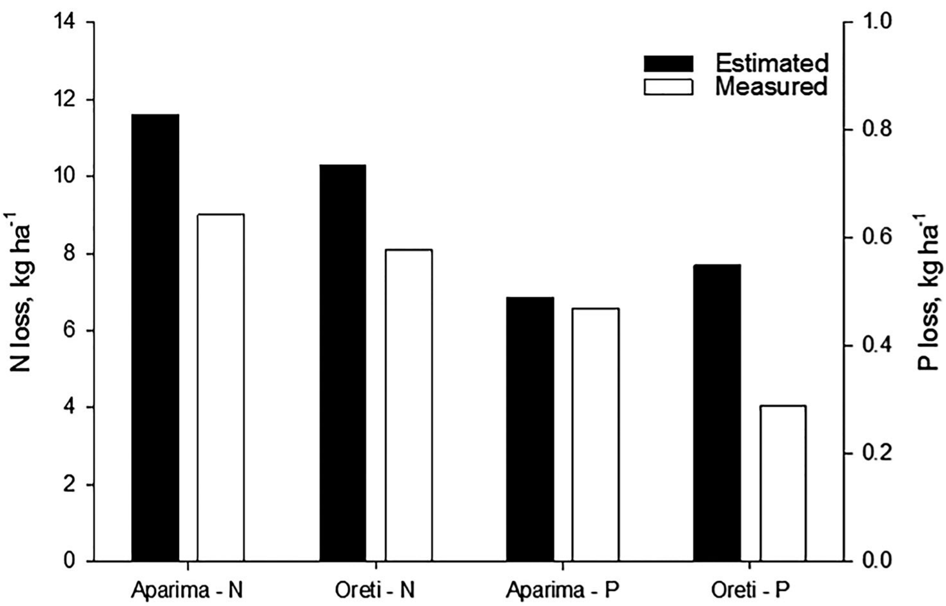

Figure 8. Comparisons of measured and modelled N and P losses in Aparima and Oreti catchments.

N attenuation between source and receptor might be underestimated by the N-attenuation layer, and secondly, the unexpectedly low delivered yields might reflect long lag times between source load generation and arrival at the monitoring site due to substantial groundwater storage and/or residence time. Corresponding research carried out in this catchment suggests that both factors might contribute to this result (Clague et al. 2019; Sarris et al. 2019a). For the Waitangi catchment we have no information of groundwater redox status and thus N attenuation. Potentially, we might expect significant N attenuation based on the amount of water (and thus load of N) transported via DGF if this groundwater was reduced or had a mixed redox status. Little N attenuation would be expected if groundwater redox status was oxic, however.

The same percentage reductions for N attenuation for each redox status were assumed for each catchment. This is a very simplistic approach as it is very likely that catchments with different hydrogeochemical characteristics will attenuate N to different degrees. The agreement that is reached for the Aparima and Oreti catchments (around 80%) and the Waiotapu catchment could readily be improved by adjustment and calibration of the N attenuation factors.

For P the story is less clear; in the case of the Oreti catchment, estimated annual losses of 0.55 kg ha^{-1} were much greater than measured losses of 0.29 kg ha^{-1}, whereas estimated and measured annual losses for the Aparima catchment were in close agreement (0.49 and 0.47 kg ha^{-1}, respectively). Some attenuation can be expected as P is transported through the surface water network, with plant uptake, sediment deposition and P sorption removing some of the P delivered from neighbouring land. However, it is unclear why there should be good agreement for the Aparima catchment, yet poor for Oreti. Plausible explanations could include over-predictions of P losses from farm typologies located in the steeper headwater areas of the Oreti catchment and, conversely, under-predictions of losses for farm typologies in the Aparima catchment (where some P attenuation would be expected).

Our analysis assumed that surface runoff and artificial drainage flow pathways were the only active conduits delivering *E. coli* from pastoral land use to water (Monaghan et al. 2016). Dwivedi et al. (2016) found that 90% of *E. coli* were trapped in the soil matrix within 0.5 m of the surface, indicating that any interflow or groundwater flow pathways will not transport significant numbers of *E. coli*. In addition, there is significant removal of microbes within most groundwater systems as documented by Pang (2009), who reviewed microbial removal rates from a large number of field studies. Thus, it appears valid to link *E. coli* transfers to the two pathways considered here (Murphy et al. 2015; Dymond et al. 2016).

The application of the above assumption to the *E. coli* model generated some contrasting results in the case study catchments. Our modelling approach predicted little surface runoff in the Waiotapu (0.01% of simulated flow routed via surface runoff, see Table 4), hence the generated *E. coli* load in this catchment was very small (Figure 9; refer to the supplementary files for other catchments). This is due to large areas of the agricultural land not generating surface flows. These low predicted loads are supported by water quality monitoring showing a median concentration of only 2 mpn 100 mL^{-1} in the upper Waiotapu catchment and 130 mpn 100 mL^{-1} at the catchment outlet (LAWA 2019a, 2019b).

Surface runoff was identified as the only pathway transporting *E. coli* in the Waitangi catchment, with the greatest loads generated in close proximity to main stems of the river network. This observation was even more pronounced in the Aparima and Oreti (refer

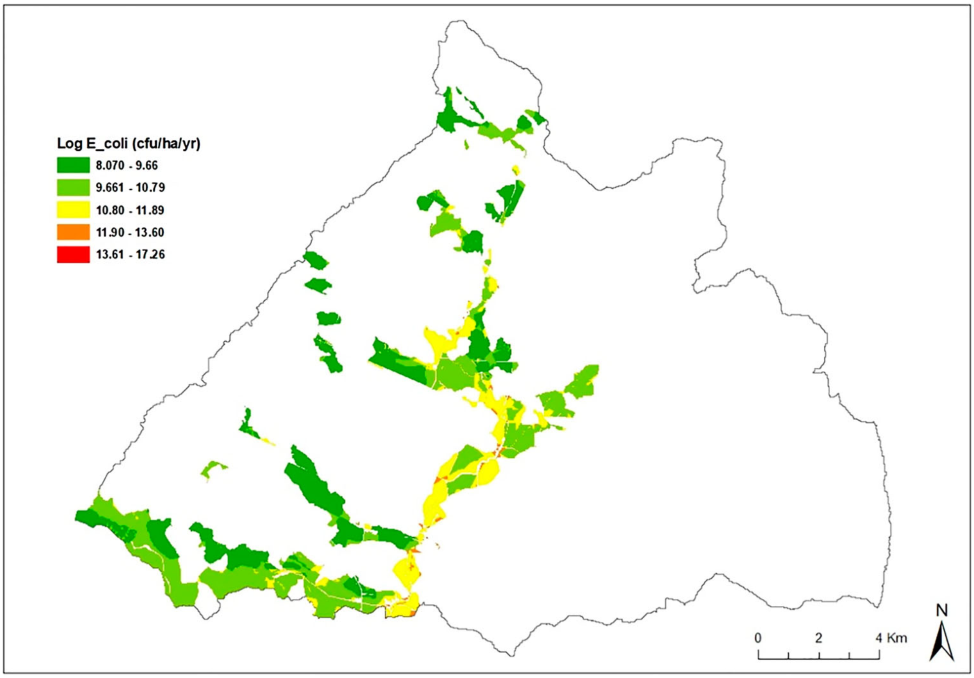

Figure 9. Estimated spatial distribution of generated *E. coli* yields (log-transformed) in the Waiotapu catchment.

Figure 10 for Oreti) catchments where the greatest loads of *E. coli* in surface runoff and artificial drainage were predicted to occur in areas close to the main river stem. This agrees with findings from a hydro-chemical modelling approach used in the Southland region that identified that *E. coli* concentrations measured in streams were strongly related to lateral drainage, artificial drainage and bypass flow (Rissmann et al. 2019). However, our findings contrast with another modelling analyses (based on stream order) that predicted that the majority (~80%) of *E. coli* loads are generated from first order streams (McDowell et al. 2017).

It should also be noted that direct inputs from farm and wild animals (Muirhead et al. 2011) represent additional and important sources of *E. coli* entering streams; these were not considered in the framework presented here. Results from this and other studies indicate that many unknowns remain with regard to modelling faecal microbe inputs to catchment waterways (Ferguson et al. 2007; Cho et al. 2016).

Benefits and limitations of the framework developed

A list of the benefits and limitations of the framework is presented in Table 5. While the framework provides a platform for consistent assessment of catchments across NZ, a lack of availability of consistent information and datasets can severely impact its development and use. The framework was designed for national scale application using national scale databases. However, the availability and consistency of data within these national scale databases varied across the country. For instance, the Waitangi catchment lacks a detailed

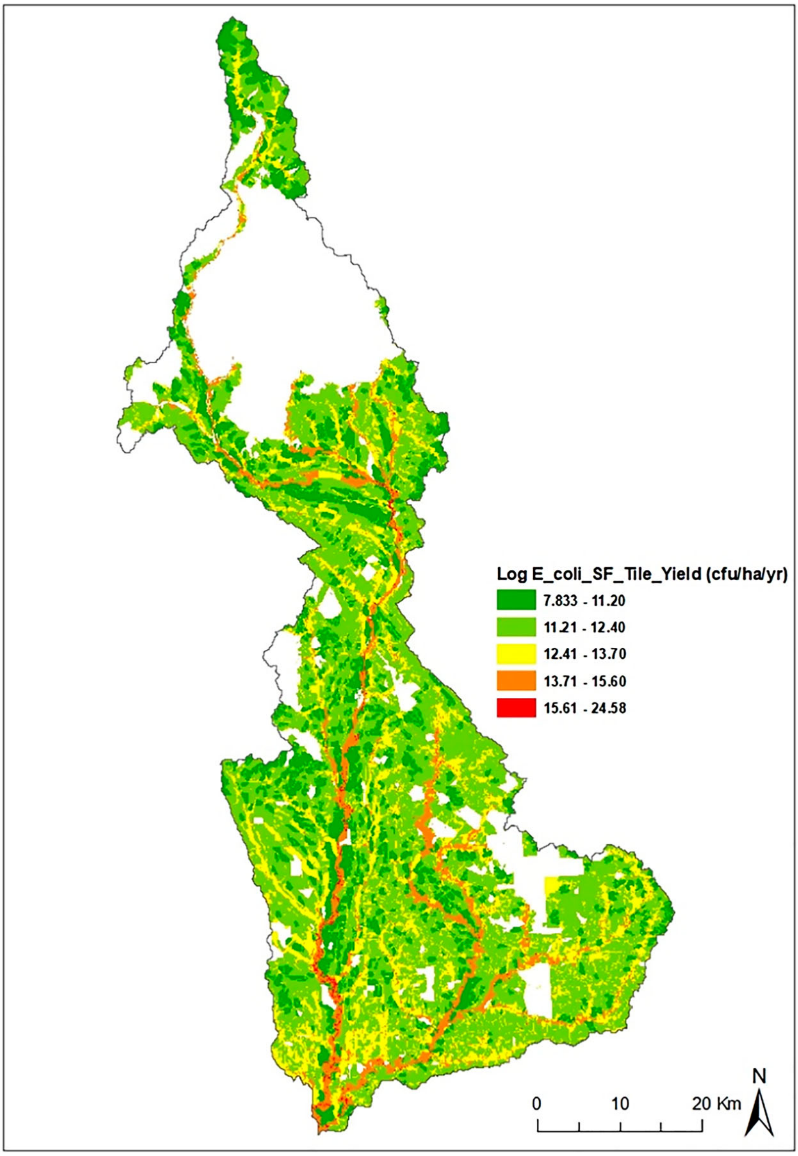

Figure 10. Estimated spatial distribution of *E. coli* yields (log-transformed) in tile drainage in the Oreti catchment.

soil map (S-Map) and an N-attenuation spatial layer. Similarly, the two Southland catchments, Oreti and Aparima lack a detailed artificial drainage layer map, which has an impact on artificial drainage and flow partitioning. Future framework development should address these data consistency and gap issues, which was not done in the current work.

The framework in its current form does not consider legacy and lags issues associated with timing and magnitude of water and contaminant storage and release from land. This shortcoming of the framework was evident in Waiotapu catchment, a groundwater

Table 5. Benefits and limitations of the framework approach.

Scientific advancement applied in the framework	Advantages of this inclusion	Limitations of this inclusion
Flow partition using a hydrology model	• Provides an approximation of transport pathways and thus the potential effectiveness of management interventions that target specific flow pathways (e.g. riparian buffers will only intercept surface flow, not artificial drainage)	• Requires high resolution data to partition flows and data on flows routed through individual flow pathways to validate the partitioned flows, which are seldom collected at catchment scales • Limited data availability in representing the differences in temporal linkages between land and water via various flow pathways • Ability of the hydrology model in simulating key surface and ground water transport processes
Inclusion of farm typology data to derive annual source yields of N and P from pastoral and non-pastoral landscape	• Enables the framework to operate without detailed land use description. • Generated yields are related to the productive capacities and landscape vulnerabilities of different locations within a catchment	• The spatial resolution of typology-derived yields is coarse compared to yields modelled using actual land use data and management information (if these data are available)
Inclusion of N attenuation in deep groundwater flow pathways	• Enables a better understanding N loads delivered to the stream network, as opposed to the generated loads	• Requires knowledge of anoxic state of groundwater in catchments and the proportion of generated N transferred through the pathway • Lags in groundwater transport times and legacy N can result in an erroneous estimation of attenuation capacities of groundwater systems • As the framework does not include in-stream N attenuation, differences in generated and delivered N loads may all be attributed to groundwater attenuation
Inclusion of multiple contaminants N, P and faecal indicator organisms in one framework	• Eliminates the need to vary models for each contaminant • Ability to maintain the same catchment hydrological behaviour for all three contaminants	• May not be as accurate as a dedicated contaminant model

dominated catchment. The framework overestimated the N loads at the catchment load which could be attributed long groundwater (hence N) residence times in the catchment.

Since N and P yield estimates are available at annual scale, the framework uses an annualised flow partition value for each pathway. This annual lumping of flow pathway partition values does not represent the differences in contaminant transport processes during high and low flow periods. Many field studies have reported that the majority of contaminant transport occur during a minority of storm events (e.g. Hooper et al. 1990; Pionke et al. 2000).

Conclusions

A simplified flow partition approach, taking into account catchment physical characteristics, meteorological and hydrological drivers, was used to model transfers of nitrogen (N), phosphorus (P) and *E. coli* from land to water in four case study catchments that varied both hydrologically and climatically. This approach was undertaken using available national scale spatial data, such as a 30-m digital elevation model, geology layers and soil and land cover information. Flows estimated based on a semi-distributed hydrology model offered a first approximation of flow partition via surface and subsurface pathways. The model calibration process needed expert guidance and data and information from previous studies to reduce the error and uncertainty caused by equifinality, where multiple potential solutions are possible for the same question; in the absence of such guidance, relying solely on input precipitation and measured flows at catchment outlets could lead to uncertainty in process representation and pathway contributions. Estimated pathway flows were aggregated at an annual scale, which meant that storm event dynamics were lost due to this averaging. Whilst recognising the limitations of this simplified approach to flow modelling, we believe it gives useful insight into the hydrological behaviour of large catchments and provides an improved and logical framework that can describe transfers of N, P and *E. coli* to water.

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ORCID

M. S. Srinivasan http://orcid.org/0000-0003-0555-235X
Richard W. Muirhead http://orcid.org/0000-0002-0913-561X
Shailesh K. Singh http://orcid.org/0000-0002-3521-3917
Ross M. Monaghan http://orcid.org/0000-0001-9469-2770
Roland Stenger http://orcid.org/0000-0003-0846-3205
Murray E. Close http://orcid.org/0000-0002-2245-4148
Andrew Manderson http://orcid.org/0000-0003-2659-7071
John J. Drewry http://orcid.org/0000-0002-8781-2604
Diana Selbie http://orcid.org/0000-0003-3825-5941
Roger Hodson http://orcid.org/0000-0002-4659-4487

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