

Water Quality in New Zealand Rivers

Modelled Water Quality State

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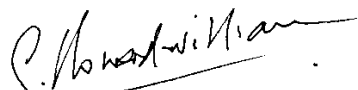
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Executive summary

This report provides model-based predictions of water quality state for each of ~ 560,000 unique river segments that comprise New Zealand's national river network, using data for the period 2009-2013. A comparable report was produced in 2010 using data for the period 2003-2007. This report is the second in a series of reports prepared for the Ministry for the Environment on national-scale state and trends in freshwater quality. The first report provided site-specific water quality state and trends for several hundred river and lake monitoring sites operated by Regional Councils and NIWA. The river water quality data acquired and processed for the first report were used in the current report.

The predicted water quality values in the current report were generated using Random Forest (RF) models. The RF empirical modelling method predicts the values of response variables using a suite of predictor variables and a dataset of observations (the 'training data'). RF models are an advanced form of regression-tree models. Single regression trees do not identify the optimum tree structure (i.e. the most accurate predictions) and they are sensitive to small changes in the observational data. To overcome these problems, RF modelling employs an ensemble of trees (a forest) and makes predictions based on the average of all trees. RF models have several additional properties that make them suitable for use in situations where the observational data are heterogeneous and the predictor variables are inter-correlated (as is often the case in water quality analyses); they require no assumptions about data distributions to be met, they are minimally affected by multi-collinearity among predictor variables, and they cannot be over-fitted.

An RF model was developed for each of eight water quality variables: nitrate-nitrogen (NO₃N), ammoniacal nitrogen (NH₄N), total nitrogen (TN), dissolved reactive phosphorus (DRP), total phosphorus (TP), visual clarity (CLAR), *Escherichia coli* (ECOLI), and the macroinvertebrate community index (MCI). The predictor variables consisted of 32 variables for which georeferenced data are stored in the River Environment Classification geodatabase. These predictor variables were selected to represent climatic, geological, topographic, land cover, and hydrological conditions in New Zealand rivers and their catchments.

The observational data used in the RF models consisted of site median values from monthly and quarterly measurements (and annual invertebrates for MCI scores) for the period 2009-2013. These data came from 354-586 monitoring sites (depending on the variable). The sites are reasonably well-distributed across the North and South Islands, with some gaps in inaccessible areas. To assess the degree to which the monitoring sites used for observational data represent the range of environmental conditions present in New Zealand, we compared histograms of the distributions of predictor variable values for the monitoring sites, with the distributions of the same variables for all river segments in New Zealand. The monitoring sites were reasonably representative, with moderate over-representation of low-elevation, low-gradient catchments with large proportions of intensive agricultural land cover.

The RF models performed well in predicting median water quality state, based on the amount of variation in the observational data explained, the congruence between observed and predicted values, low model bias (tendency to over- or under estimate), and low prediction uncertainty.

The most important predictor variables for the nutrient models and the CLAR and ECOLI models for river segments were the proportions of intensive agricultural and urban land cover in catchments and catchment elevation and slope. For the MCI model, the most important predictor variables were

the proportions of native forest and urban land cover and catchment elevation. Collectively, the models suggest that chemical and microbiological water quality is most severely compromised in low-elevation, low-gradient land under intensive land use.

National maps of predicted median nutrient and ECOLI concentrations have relatively high values in low-elevation areas on the east coasts of the North and South Island, and in the inland Waikato, Wairarapa Valley, Rangitikei-Manawatu coastal plain, Taranaki Ring Plain, and Auckland Region. Predicted nutrient and ECOLI concentrations are generally low in major mountain ranges, in large areas of the Department of Conservation estate and in other native forest-dominated areas. Predicted DRP and TP concentrations appear to be elevated in rivers draining phosphorus-rich Tertiary mudstone and volcanic ash on the North Island, which suggests that parent geology affects large scale patterns in river DRP and TP. However, the effects of geology are likely to be inter-correlated with land use and topography. Geographic patterns in predicted CLAR and MCI scores are generally the reverse of the patterns for chemical and microbial water quality, with high values in mountain ranges and Department of Conservation estate, and low values in areas dominated by intensive agriculture and urban land cover.

1 Introduction

River water quality is characterised by the recent state and trends in several variables that are measured at monitoring sites distributed across New Zealand. The sites are monitored as part of the State of Environment (SOE) programmes operated by Regional Councils and unitary authorities and the National River Water Quality Network (NRWQN) operated by NIWA.

This document is the second of two reports updating national river water quality state in New Zealand, using data from the council SOE programmes and the NRWQN. The first report “Analysis of water quality in New Zealand lakes and rivers” provided information on water quality state and trends for individual river and lake monitoring sites (Larned et al. 2015). The updated river dataset used in the state analyses of the first report contained measurements for eight physical, chemical, microbiological and macroinvertebrate variables from 365 to 577 sites, for the 2009-2013 period. Site-specific water quality state in the first report was based on median variable values for that five-year period.

In the current report, we developed Random Forest (RF) models to relate spatial variation in the same eight water quality variables used in the previous report to a large suite of environmental predictor variables. The predictor variables represent climatic, geological, topographic, land cover, and hydrological conditions in New Zealand rivers and their catchments. The RF models were used to predict river water quality at un-monitored locations, and to produce spatially continuous maps of predicted water quality variation. These maps comprise a high level statistic that describes predicted patterns in water quality at the national scale.

One of the primary purposes of predictive RF models is to provide large-scale water quality assessments that are more representative of the true patterns of water quality than assessments based on aggregated data from multiple monitoring sites. The latter approach can lead to conclusions about water quality patterns that are biased by the non-random locations of monitoring sites. Previous analyses have shown that the aggregate network of river water quality monitoring sites in New Zealand is over-represented by sites in catchments dominated by pastoral land cover and under-represented by sites in catchments dominated by native forest (Larned and Unwin 2012). This non-representative distribution of sites can produce biased results when multiple environmental classes are merged. Using RF models to predict water quality state in all river reaches in New Zealand can reduce this problem.

In this report, we provide detailed methods for using RF models to predict river water quality state across the heterogeneous New Zealand environment. The methodological steps include preparation of the water quality state data, selection of environmental predictor variables, assessment of site representativeness, the RF modelling process, and assessments of model performance. In the results section, we present maps of national predictions of river water quality, identify important predictor variables and quantify model performance. In the discussion section, we compare the current RF models with previous models of river water quality state and comment briefly on uncertainty in RF models and alternative modelling methods.

2 Data

2.1 River water quality data

The monitoring sites and data used in the Stage 1 study to analyse water quality state (Larned et al. 2015) were also used for the current study. The water quality data consisted of measurements of eight physical, chemical, microbiological and invertebrate variables from river monitoring sites in council SOE networks and the NRWQN sites (Table 2-1). Detailed methods for processing the water quality data are given in Larned et al. (2015). The monitoring sites had the following properties: 1) less than 50% of the values for a variable were censored; 2) values for at least 90% of monthly or quarterly sampling dates were available, including imputed values; 3) at least 30 values were distributed over four of the five years from 2009 to 2013. In contrast, the invertebrate data come from annual monitoring and there were no censored data. The sole rule for including invertebrate monitoring sites was that data were available for at least four of the five years from 2009 to 2013.

The Stage 1 study used the original version of the River Environment Classification (REC1; Snelder and Biggs 2002) as a spatial framework to provide environmental context for the analysis. In the current study, we used a recently updated version of the REC, referred to as REC2 (see Section 2.2 for details). All monitoring sites from the Stage 1 study were projected on to the REC2 digital river network, then manually checked. At this step, eight sites were omitted because they could not be reliably associated with the network location reported by the corresponding council¹. In the final dataset used for RF modelling, between 364 and 586 sites met the inclusion criteria for at least one of the eight water quality variables (Table 2-1).

The geographic distribution of river monitoring sites used for modelling is shown in Fig. 2-1. The sites are reasonably well-distributed, although there are gaps in the central North and central South Islands. There is a high degree of overlap among the sites used for physical, chemical and microbiological water quality monitoring, as some or all of the corresponding variables are measured at each site in council SOE programmes. There is less overlap among sites used for invertebrate monitoring; several councils operate separate programmes for monitoring physical-chemical water quality and invertebrates, with variable levels of site overlap between programmes.

¹ Excluded sites included three water quality sites: ARC-45505, ECAN-SQ00180 and ECAN-SQ00225 and five invertebrate sites; ECAN-SQ00038, ECAN-SQ00180, ECAN-SQ00225 GWRC-RS54 and NCC-33.

Table 2-1: River water quality variables, measurement units and site numbers used to develop Random Forest models.

Variable type	Variable	Abbreviation	Units	Number of monitoring sites
Physical	Visual clarity	CLAR	m	454
Chemical	Ammoniacal nitrogen	NH4N	mg/m ³	364
	Nitrate-nitrogen	NO3N	mg/m ³	586
	Total nitrogen (unfiltered)	TN	mg/m ³	354
	Dissolved reactive phosphorus	DRP	mg/m ³	518
	Total phosphorus (unfiltered)	TP	mg/m ³	576
Microbiological	<i>Escherichia coli</i>	ECOLI	cfu/100 mL	485
Biotic Index	Macroinvertebrate Community Index	MCI	unitless	505

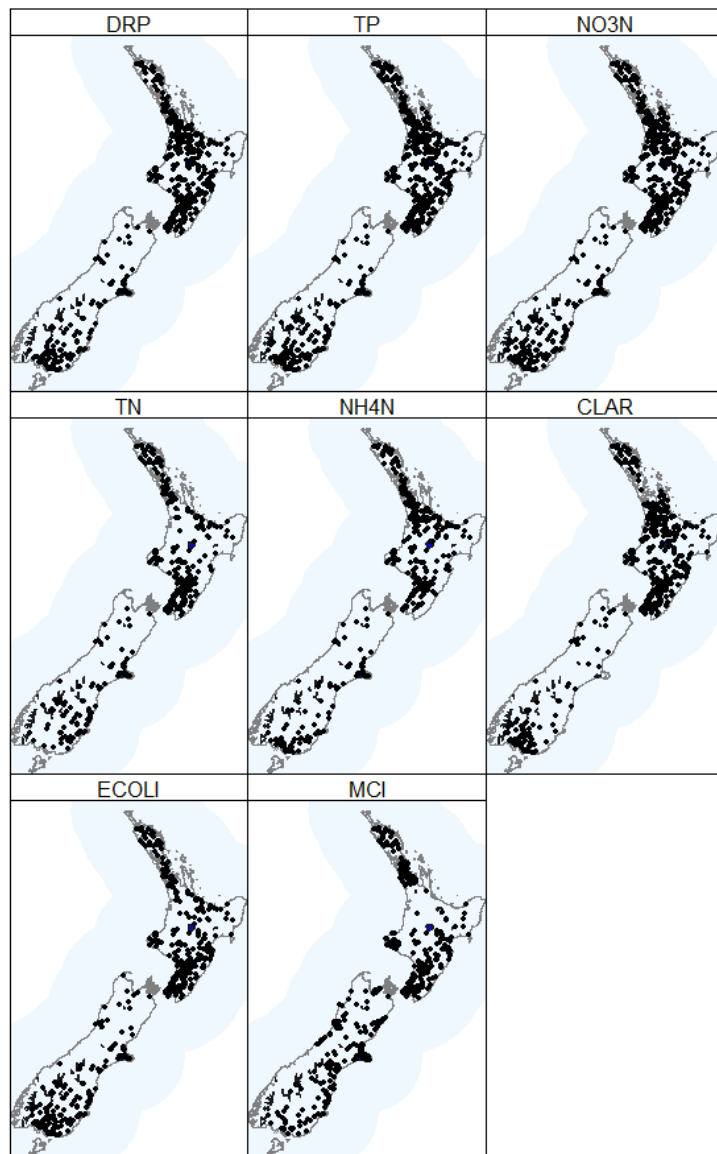


Figure 2-1: Locations of river water quality monitoring sites used for modelling the state of eight water quality variables. The locations on each panel correspond to the site numbers listed for each variable in Table 2-1.

2.2 Predictor data

The digital river network and catchment boundaries used for the REC provided the spatial framework for the RF models of river water quality state. The river network and catchment boundaries were derived from a digital elevation model (DEM) with a spatial resolution of 50 m. The digital network represents New Zealand's rivers as ~ 560,000 segments (bounded by upstream and downstream confluences) and their corresponding catchments. Each segment in the digital network has a unique identifier, the NZSegment number. The links between each NZSegment and its catchment, between adjacent NZSegments and between adjacent catchments facilitate analyses of upstream-downstream connectivity and the accumulation of catchment characteristics in the downstream direction. The digital network has been recently updated to correct errors and to improve its representation of rivers nationally; the REC geodatabase with the updated network is referred to as REC2.

In addition to the digital network, the REC2 contains spatial data layers describing the climate, topography, geology, vegetation, infrastructure and hydrology of New Zealand (<https://www.niwa.co.nz/freshwater-and-estuaries/management-tools/river-environment-classification-0>). These spatial data are used to link each NZSegment to a large number of attributes that describe the environmental characteristics of the segment and its catchment. Catchment land cover in REC2 is derived from the national Land Cover Database-3 (LCDB3) which differentiates 33 categories based on analysis of satellite imagery from 2008 (Iris.scinfo.org.nz). Descriptions of catchment regolith are derived from the Land Resources Inventory (LRI) including interpretations of the LRI categories made by (Leathwick et al. 2003). Additional variables for each segment have been derived from national-scale hydrological modelling (e.g. Booker and Snelder 2012).

We selected 32 network attributes from the REC2 (Table 2-2) for predictor variables in spatial models of the eight water quality variables listed in Table 2-1. The predictor variables were selected on the basis of their predicted mechanistic or correlative relationships with water quality, and on previous experience with national scale modelling of water quality (e.g. (Unwin et al. 2010) and invertebrate communities (Clapcott et al. 2013; Leathwick et al. 2011).

Table 2-2: Predictor variables used in Random Forest models of river water quality variables. *Geological variables are based on regolith, using averages of ordinal values assigned to LRI top-rock categories by Leathwick et al. (2003). The variables usHard and usPsize characterise physical regolith conditions; usPhos and usCalc characterise regolith fertility.

Predictor variable class	Predictor variable description	Abbreviation	Unit
Geography & topography	Catchment area	usArea	m ²
	Mean annual catchment rainfall	usRain	mm
	Mean annual catchment potential evapotranspiration	usPET	mm/yr
	Estimated mean flow	MeanFlow	m ³ /s
	Segment mean elevation	segElev	m ASL
	Percentage of catchment occupied by lakes	usLakePerc	%
	Mean catchment elevation	usElev	m ASL
	Mean catchment slope	usSlope	degrees
	Distance to the coast	DistToCoast	m
	Mean segment slope	SegSlope	degrees
	Segment sinuosity (segment length divided by the straight line distance between endpoints)	Sinuosity	unitless
Climate & flow	Distance to furthest headwater segment	DistToHead	m
	Mean segment June air temperature	segTmin	degrees C x 10
	Mean segment January air temperature.	segTwarm	degrees C x 10
	Mean catchment June air temperature	usTmin	degrees C x 10
	Mean catchment January air temperature	usTwarm	degrees C x 10
	Mean catchment coefficient of variation of annual rainfall	usRainvar	mm/yr
	Mean catchment rain days > 10mm	usRainDays10	days/mo
Geology*	Mean catchment rain days > 200mm	usRainDays20	days/mo
	Mean catchment rain days > 100mm	usRainDays100	days/mo
	Mean catchment induration (hardness) of regolith	usHard	Ordinal
	Mean catchment phosphorous content of regolith	usPhos	Ordinal
Land cover	Mean catchment particle size of regolith	usPsize	Ordinal
	Mean catchment calcium content of regolith	usCalc	Ordinal
	Proportion of catchment occupied by combination of high producing exotic grassland, short-rotation cropland, orchard, vineyard and other perennial crops (LCDB3 classes 40, 30, 33)	usIntensiveAg	%
	Proportion of catchment in low producing grassland (LCDB3 class 41)	usPastoralLight	%
	Proportion of catchment in native forest (LCDB3 class 69)	usNativeForest	%
	Proportion of catchment in built-up areas, urban parkland, surface mines, dump and transport infrastructure (LCDB3 classes 1,2,6,5)	usUrban	%
	Proportion of catchment in scrub and shrub cover (LCDB3 classes 50, 51, 52, 54, 55, 56, 58)	usScrub	%
	Proportion of catchment occupied by lake and pond, river and estuarine open water (LCDB3 classes 20, 21, 22)	usWetland	%
Proportion of catchment in exotic forest (LCDB3 class 71)	usExoticForest	%	
Proportion of catchment occupied in bare or lightly-vegetated cover (LCDB3 classes 10, 12, 14, 15, 16)	usBare	%	

3 Modelling methods

3.1 Random forest models

We modelled log-transformed median values of each water quality variable (i.e. the \log_{10} of the median of the untransformed raw data) as a function of the predictor variables using RF models (Breiman et al. 1984; Breiman 2001; Cutler et al. 2007). An RF model is an ensemble of individual classification and regression trees (CART). In a regression context, CART partitions observations (in this case the individual water quality variables) into groups that minimise the sum of squares of the response (i.e. assembles groups that minimise differences between observations) based on a series of binary rules or splits that are constructed from the predictor variables. CART models have several desirable features including requiring no distributional assumptions and the ability to automatically fit non-linear relationships and high order interactions. However, single regression trees have the limitations of not searching for optimal tree structures, and of being sensitive to small changes in input data (Hastie et al. 2001). RF models reduce these limitations by using an ensemble of trees (a forest) and making predictions based on the average of all trees (Breiman 2001). An important feature of RF models is that each tree is grown with a bootstrap sample of the fitting data (i.e. the observation dataset). In addition, a random subset of the predictor variables is made available at each node to define the split. Introducing these random components and then averaging over the forest increases prediction accuracy while retaining the desirable features of CART.

An RF model produces a limiting value of the generalization error (i.e. the model maximises its prediction accuracy for previously unseen data; Breiman 2001). The generalization error converges asymptotically as the number of trees increases, so the model cannot be over-fitted. The number of trees needs to be set high enough to ensure an appropriate level of convergence, and this value depends on the number of variables that can be used at each split. We used default options that included making one third of the total number of predictor variables available for each split, and 500 trees per forest. Some studies report that model performance is improved by including more than ~ 50 trees per forest, but that there is little improvement associated with increasing the number of trees beyond 500 (Cutler et al. 2007). Our models took less than a minute to fit when using the default of 500 trees per forest.

Unlike linear models, RF models cannot be expressed as equations. However, the relationships between predictor and response variables represented by RF models can be represented by importance measures and partial dependence plots (Breiman 2001; Cutler et al. 2007). During the fitting process, RF model predictions are made for each tree for observations that were excluded from the bootstrap sample; these excluded observations are known as out-of-bag (OOB) observations. To assess the importance of a specific predictor variable, the values of the response variable are randomly permuted for the OOB observations, and predictions are obtained from the tree for these modified data. The importance of the predictor variable is indicated by the degree to which prediction accuracy decreases when the response variable is randomly permuted. Importance is defined in this study as the loss in model performance (i.e. the increase in the mean square error; MSE) when predictions are made based on the permuted OOB observations compared to those based on the original observations. The differences in MSE between trees fitted with the original and permuted observations are averaged over all trees, and normalized by the standard deviation of the differences (Cutler et al. 2007).

A partial dependence plot is a graphical representation of the marginal effect of a predictor variable on the response variable, when the values of all other predictor variables are held constant. The

benefit of holding the other predictors constant (generally at their respective mean values) is that the partial dependence plot effectively ignores their influence on the response variables. Partial dependence plots do not perfectly represent the effects of each predictor variable, particularly if predictor variables are highly correlated or strongly interacting, but they do provide an approximation of the modelled predictor-response relationships that are useful for model interpretation (Cutler et al. 2007).

RF models can include any of the original set of predictor variables that are chosen during the model fitting process. Inclusion of marginally important and correlated predictor variables does not degrade the performance of the RF models. However, these predictor variables may be redundant (i.e. their removal does not affect model performance) and their inclusion can complicate model interpretation. We used a backward elimination procedure to remove redundant predictor variables from the initial 'saturated' models (i.e. models that included any of the original predictor variables). The procedure first assesses the model error (MSE) using a 10-fold cross validation process. The predictions made to the hold out observations during cross validation are used to estimate the MSE and its standard error. The model's least important predictor variables are then removed in order, with the MSE and its standard error being assessed for each for each successive model. The final, 'reduced' model is defined as the model with the fewest predictor variables whose error is within one standard error of the best model (i.e. the model with the lowest cross validated MSE). This is equivalent to the "one standard error rule" used for cross validation of classification trees (Breiman et al. 1984).

An alternative approach is to choose the model with the smallest error. We used the former procedure as it retains fewer predictor variables than the latter procedure, while achieving an error rate that is not different, within sampling error, from the "best solution". Importance levels for predictor variables were not recalculated at each reduction step to avoid over-fitting (Svetnik et al. 2004).

We note that, because fitting a RF model involves randomly selecting observations and predictor variables throughout the fitting process, successive models fitted to the same data set will exhibit subtle differences in structure and diagnostics such as total explained deviance, MSE, partial dependence plots, and the order of predictor importance. In the current study, the variability in model error between individual fits of the model for each water quality variable were within the reported model performance (see Section 3.2).

All calculations were performed in the R statistical computing environment (R Development Core Team 2009) using the *randomForest* package and other specialised packages.

3.2 Model performance

Model performance was assessed by comparing observations with independent predictions (i.e. sites that were not used in fitting the model), which were obtained from the out-of-bag (OOB) samples. We summarised the models using four statistics; regression R^2 , Nash-Sutcliffe Efficiencies (NSE), bias and root mean square deviation (RMSD).

The regression R^2 value is the coefficient of determination derived from a regression of the observations against the predictions. The R^2 value shows the proportion of the total variance explained by the regression model (Piñeiro et al. 2008). However, the regression R^2 is not a complete description of model performance. The NSE (Nash and Sutcliffe, 1970) provides a measure of overall model performance by indicating how closely a plot of observed versus predicted values lies to the

1:1 line (i.e. the degree to which two sets of values coincide). NSE values range from $-\infty$ to 1. An NSE of 1 corresponds to a perfect match between predictions and the observed data, an NSE of 0 indicates that the model predictions are as accurate as the mean of the observed data; and an NSE < 0 indicates that the observed mean is a better predictor than the model. Model bias measures the average tendency of the predicted values of water quality variables to be larger or smaller than the observed values. Positive values indicate underestimation bias and negative values indicate overestimation bias (Moriassi et al. 2007). The RMSD is a measure of the characteristic model uncertainty. RMSD is mean deviation of predicted values with respect to the observed values (distinct from the standard error of the regression model).

3.3 Representativeness of monitoring sites used in RF models

A graphic comparison was used to gauge how well the monitoring sites used to fit the RF models represented environmental variation at the national scale. Here, representativeness refers to the degree to which the distribution of monitoring sites over the range of an environmental predictor variable matches the distribution of all network segments over the range of the same environmental variable. Poor representativeness can reduce accuracy in model predictions because certain combinations of environmental conditions are not represented in the fitting data.

Histograms of the proportions of monitoring site numbers over the ranges of the 12 most important predictor variables in the RF models (i.e. the predictors with the greatest explanatory power) were visually compared with histograms of the proportions of all network segments over the same predictor variables. Two sets of comparable histograms were derived. The first represented data from all monitoring sites that included at least one water quality variable, except MCI (596 sites). The second set of comparable histograms represented the 505 invertebrate monitoring sites that were used for modelling MCI scores. Separate histograms were constructed due to the limited overlap in physical-chemical water quality and invertebrate monitoring sites, as noted in Section 2.1.

Note that representativeness of monitoring sites is different from model bias, which is defined in Section 3.2. Model bias is a measure of systematic error in model predictions (i.e., over- or under-estimation).

3.4 Model predictions

Predictions are made with RF models by “running” new cases down every tree in the fitted forest and averaging the predictions made by each tree (Cutler et al. 2007). The models in this study were fitted to \log_{10} -transformed water quality data. When these models are back-transformed, the model error term no longer has a mean of zero. Ignoring this results retransformation bias, i.e. predictions that systematically underestimate the response. We corrected the retransformation bias using the smearing estimate (S) developed by Duan (1983):

$$S = \frac{1}{n} \sum_{i=1}^n 10^{\hat{\varepsilon}_i} \quad (\text{Equation 1}),$$

where $\hat{\varepsilon}$ are the residuals of an RF model. The predictions were back-transformed by raising them to the power of 10, then corrected for retransformation bias by multiplying by S . The back-transformed and corrected predictions for all river segments in New Zealand were projected on a single national map for each water quality variable.

4 Results

4.1 Model performance

The RF models for all water quality variables performed well, as indicated by the following statistics: $R^2 > 0.5$, $NSE > 0.5$, and $RMSD < 0.4$ for all variables except MCI, for which $RMSD = 10.4$ (Table 4-1). Bias in the RF models was low as indicated by the close match between the line representing the regression of the observed versus predicted values (red dashed line in Figure 4-1) and the one-to-one line (blue solid line in Figure 4-1). The close match between the regression and one to one line also indicates that the models are consistent (i.e. that low or high values are not under or over-estimated). Based on NSE values, the ECOLI, TN and NO₃N models had the best overall performance, NH₄N, DRP and CLAR models had the worst overall performance, and the MCI and TP models had intermediate performance.

Table 4-1: Performance of the water quality models. Performance was determined using independent predictions (i.e. sites that were not used in fitting the models) generated from the out-of-bag observations. Regression R^2 = coefficient of determination, NSE = Nash-Sutcliffe efficiency, RMSD = root mean square deviation). Units for RMSD and bias are the log₁₀ transformed units of the respective water quality variables except for MCI, for which RMSD and bias are based on non-transformed data.

Model (water quality variable)	Number of sites	Regression R^2	NSE	RMSD	Bias
CLAR	454	0.59	0.58	0.20	0.000
DRP	518	0.58	0.58	0.28	-0.002
ECOLI	485	0.77	0.77	0.32	-0.008
NH ₄ N	364	0.51	0.51	0.31	-0.011
NO ₃ N	586	0.71	0.70	0.39	-0.008
TN	353	0.76	0.76	0.23	-0.005
TP	576	0.67	0.66	0.23	-0.001
MCI	505	0.69	0.68	10.41	-0.081

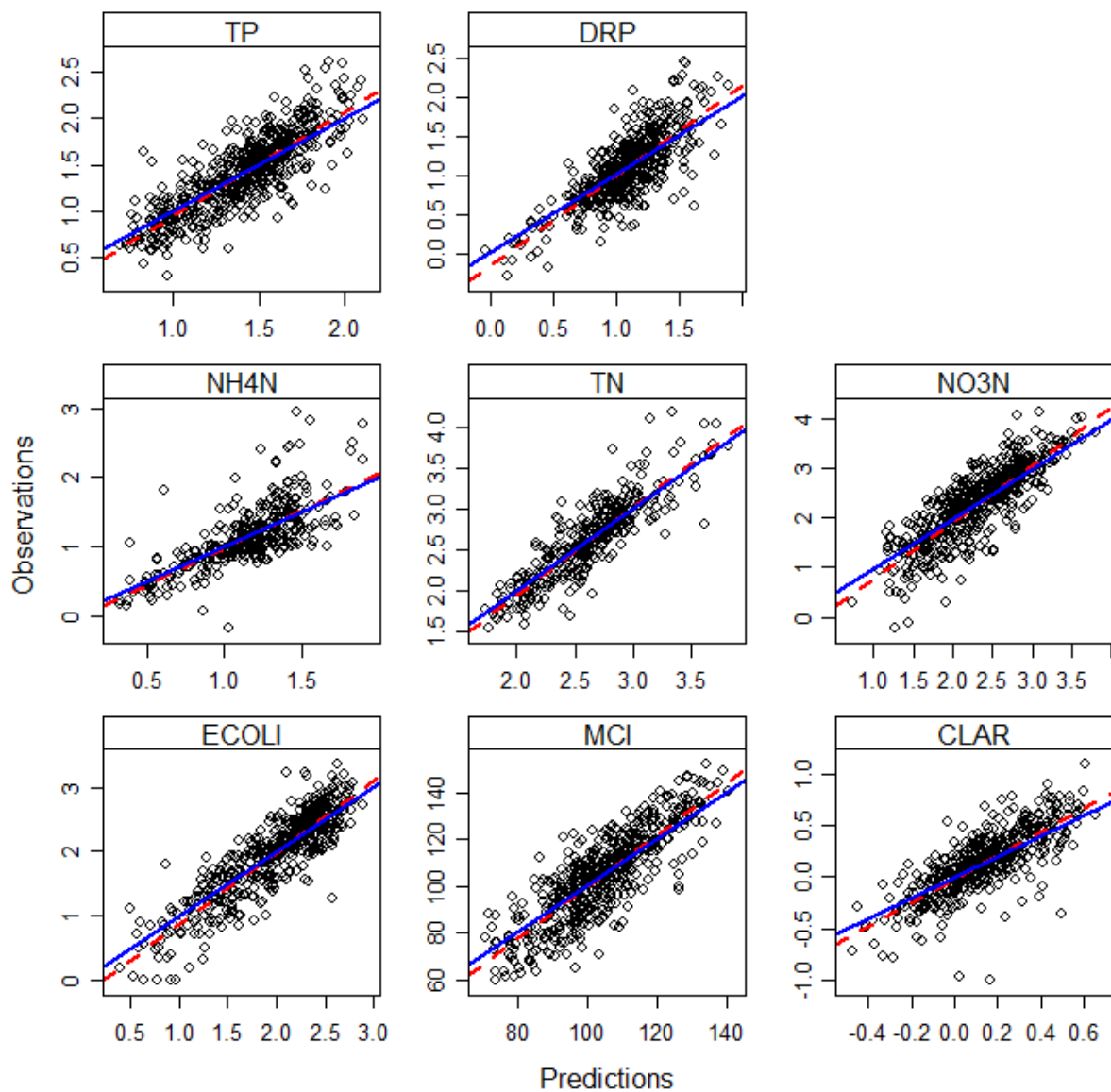


Figure 4-1: Comparison of observed water quality versus values predicted by the random forest models. Note that the observed values are plotted on the Y-axis and predicted values on the X-axis, following Piñeiro et al. (2008). Red dashed line: best fit linear regression of the observed and predicted values. Blue solid line: one-to-one line. Units are the log10 transformed units of all water quality variables except for MCI, which uses non-transformed values.

4.2 Monitoring site representativeness

The distributions of river water quality and MCI monitoring sites across the environmental gradients defined by 12 predictor variables were generally consistent with the distribution of all segments in the river network across the same gradients (Fig.s 4-2 and 4-3). The predictor variables shown in the histograms in Figures 2-3 and 2-4 were those subsequently found to be important to the RF models.

There were several cases of moderate over- and under-representation of monitoring sites compared to the river network. Water quality sites were over-represented in environments characterised by low segment elevations (segElev), low catchment elevations (usElev) and low catchment slopes (usSlope) (Figure 4-2). Water quality sites were under-represented in catchments with high proportions of native forest land cover (usNativeForest), and catchments with low proportions of intensive agricultural land cover (usIntensiveAg).

Invertebrate monitoring sites were over-represented in catchments with high proportions of urban land cover (usUrban) and high intensity agricultural land cover (usIntensiveAg), and under-represented in catchments with high proportion of native forest land cover (usNativeForest) (Fig. 4-3). Invertebrate sites were also over-represented in low gradient rivers (segSlope).

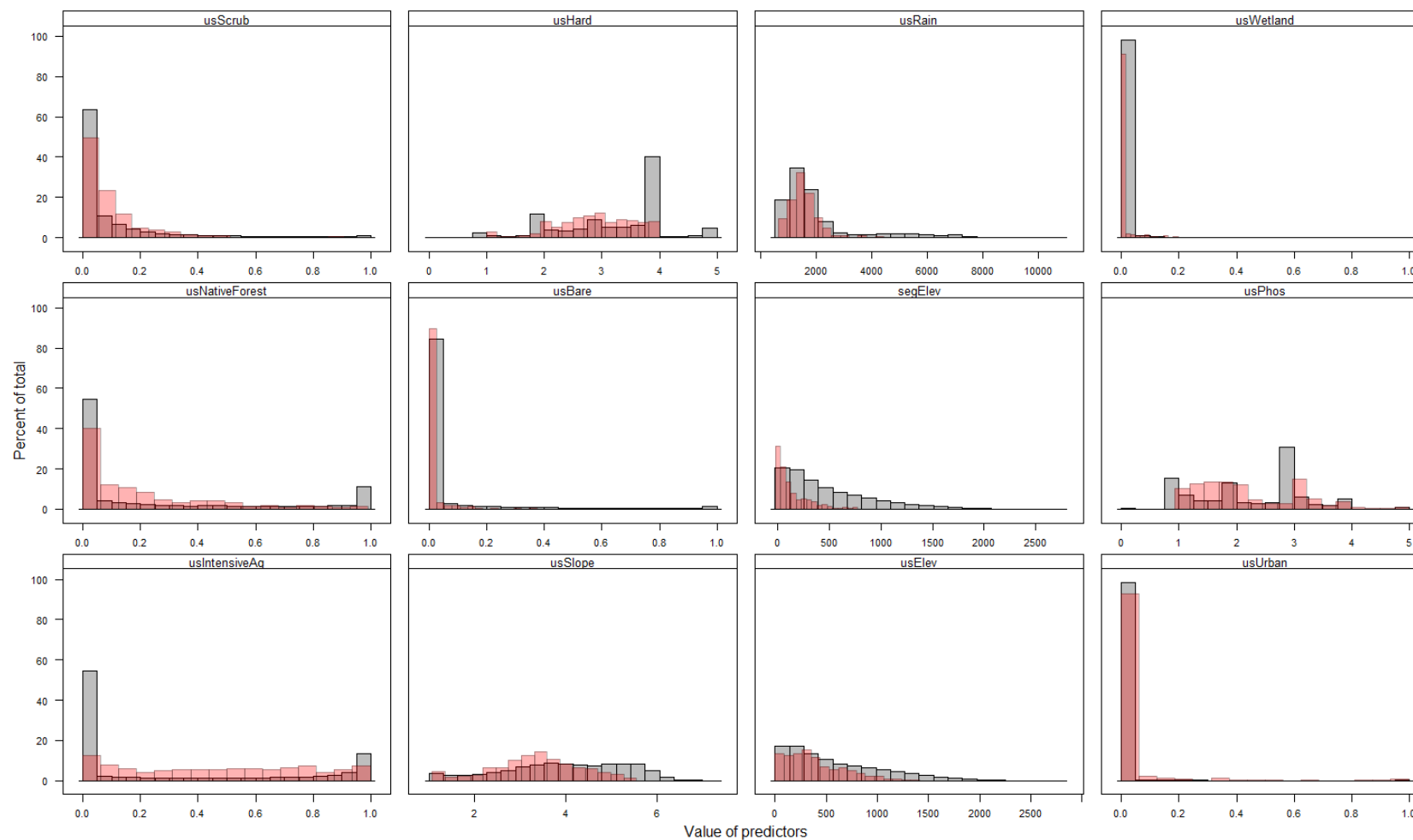


Figure 4-2: Histograms showing the distributions of predictor variable values for all segments in the digital river network (grey histograms) and the water quality sites used for RF models (red histograms). Similarities in the distributions shown in the two histograms in each panel provide an indication of the degree to which environmental variation across the monitoring sites represents environmental variation across the New Zealand river network; complete representativeness would be indicated by exact matches between the histograms. The twelve predictor variables shown in the figure were the most important overall predictors in the RF models, with the exception of MCI (due to large differences between the locations of invertebrate monitoring sites and sites used for other water quality variables).

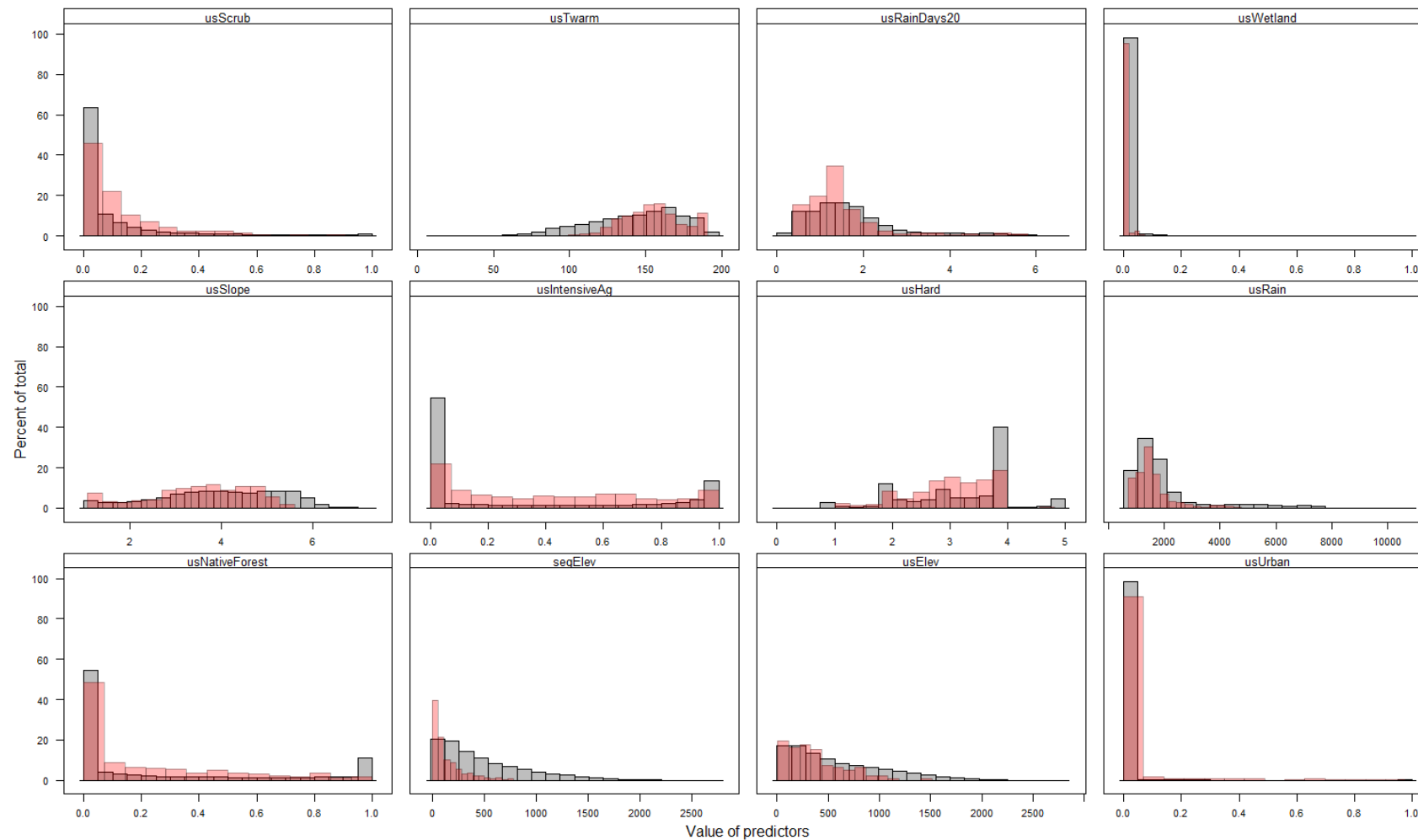


Figure 4-3: Histograms showing the distributions of predictor variable values for all segments in the digital river network (grey histograms) and for the invertebrate monitoring sites used for RF models of MCI (red histograms). Similarities in the distributions shown in the two histograms for each predictor variable provide an indication of the degree to which environmental variation across the monitoring sites represents environmental variation across the New Zealand river network. The twelve predictor variables shown in the figure were the most important in RF models of MCI.

4.3 Modelled relationships

The predictor variables with high importance in all RF models reflected strong associations between water quality and land use and catchment topography. The predictor *usIntensiveAg*, which indicates the proportion of the catchment that is occupied by intensive agriculture land cover, had the highest overall importance (Table 4-2). This predictor was ranked first, second or third highest in importance in the RF models of all water quality variables except MCI (ranked fifth) and DRP (ranked 19th). The partial plots indicated that CLAR and MCI decreased with increasing values of *usIntensiveAg* and the values of all other water quality variables increased (Fig.s 4-4 and 4-5).

The predictors *usSlope* and *usElev*, which represent the mean slope and mean elevation of the catchment, had the second and third highest overall importance ranks (Table 4-2). The partial plots indicated that CLAR and MCI increased with increasing values of *usSlope* and *usElev* and the values of all other water quality variables decreased (Fig.s 4-4 and 4-5). The associations with *usIntensiveAg* and elevation are consistent with recent evaluations of environmental patterns in river water quality (e.g. Larned et al. 2004; 2016; Unwin et al. 2010).

The proportion of the catchment occupied by urban land cover (*usUrban*) had the fourth highest overall ranking. Predicted ECOLI and nutrient concentrations increased and MCI scores decreased with increasing values of *usUrban* (Fig.s 4-4 and 4-5). This association is consistent with observations of negative correlations between urban land-cover and water quality state (Larned et al. 2004; 2016).

For the MCI model, the highest ranked predictor was *usNativeForest*, which characterises the proportion of the catchment that is occupied by late-successional native forest (Table 4-2). Predicted MCI scores increased with increasing values of *usNativeForest* (Fig. 4-5). Segment elevation was the second highest ranked variable for the MCI model (Table 4-2) and the partial plots indicated that MCI scores increase with increasing elevation (Fig. 4-5).

The predictors *usBare*, *usPhos*, *usHard* and *usPsize* had relatively high importance in the water quality RF models (ranks of 5th, 9th, 11th and 12th respectively (Table 4-2)). These predictors indicate that the regolith of the catchment is associated with water quality state. The values of most water quality variables decreased with increasing values of *usBare*, *usHard* and *usPsize* (Fig. 4-4). These patterns suggest that water quality generally declines as regolith fertility increases.

The mean annual catchment rainfall (*usRain*) was the 10th most important overall predictor for the water quality variables and was the 7th most important predictor for the MCI model. The values of CLAR and MCI increased with increasing *usRain*, and the values of all other water quality variables decreased (Fig.s 4-4 and 4-5). These results suggest that there is a moderately strong positive association between water quality state and catchment rainfall. The mechanisms that drive this association may include solute dilution and sustained low water temperatures. The frequency of high intensity rainfall (*usRainDays100*, *usRainDays20* and *usRainDays10*) had relatively high importance in the models of CLAR and MCI (Table 4-2), with MCI and CLAR values increasing with increasing values of these predictors (Fig.s 4-4 and 4-5).

Table 4-2: Rank order of importance of predictor variables retained in the random forest models for at least one water quality variable. Blank cells indicate that the predictor was not included in the reduced model. The predictor variables in the first column are listed in descending order of the median of the rank importance over all eight models.

Predictor variable	CLAR	DRP	ECOLI	NH4N	NO3N	TN	TP	MCI
usIntensiveAg	1	17	1	3	1	1	2	6
usSlope	7	1	5	2	2	2	1	5
usElev	2	8	2	1	6	3	6	3
usUrban			8	4	7	5		4
usNativeForest	5			7	11	6	8	1
usBare	9	2	6	8			3	30
segElev	10		9	6				2
usPhos	4	7	4	11	8		11	14
usScrub		16			4	8		9
usHard		9		16	19		5	7
usRain	14	3		10	9	9	7	8
usWetland		5	7		16			12
usPsize		4	12		10		10	18
usTmin	12	6	10	12		7	4	20
DistToCoast		11		5				27
usRainvar	3		3	9	15		13	24
segTmin		10		15	5		12	29
usTwarm	16	13			14	11	9	10
MeanFlow	15	12	11					22
DistToHead	11							17
usRainDays20		14			20			11
usRainDays10		20	14		17		14	13
usExoticForest		15	15		3	4		31
segTwarm	6	19			12		15	19
usRainDays100	8							23
usPET		18			13		16	16
SegSlope					21			15
usLakePerc			13		18			28
usPastorallight		22	16	13	22	10		25
usCalc				14				26

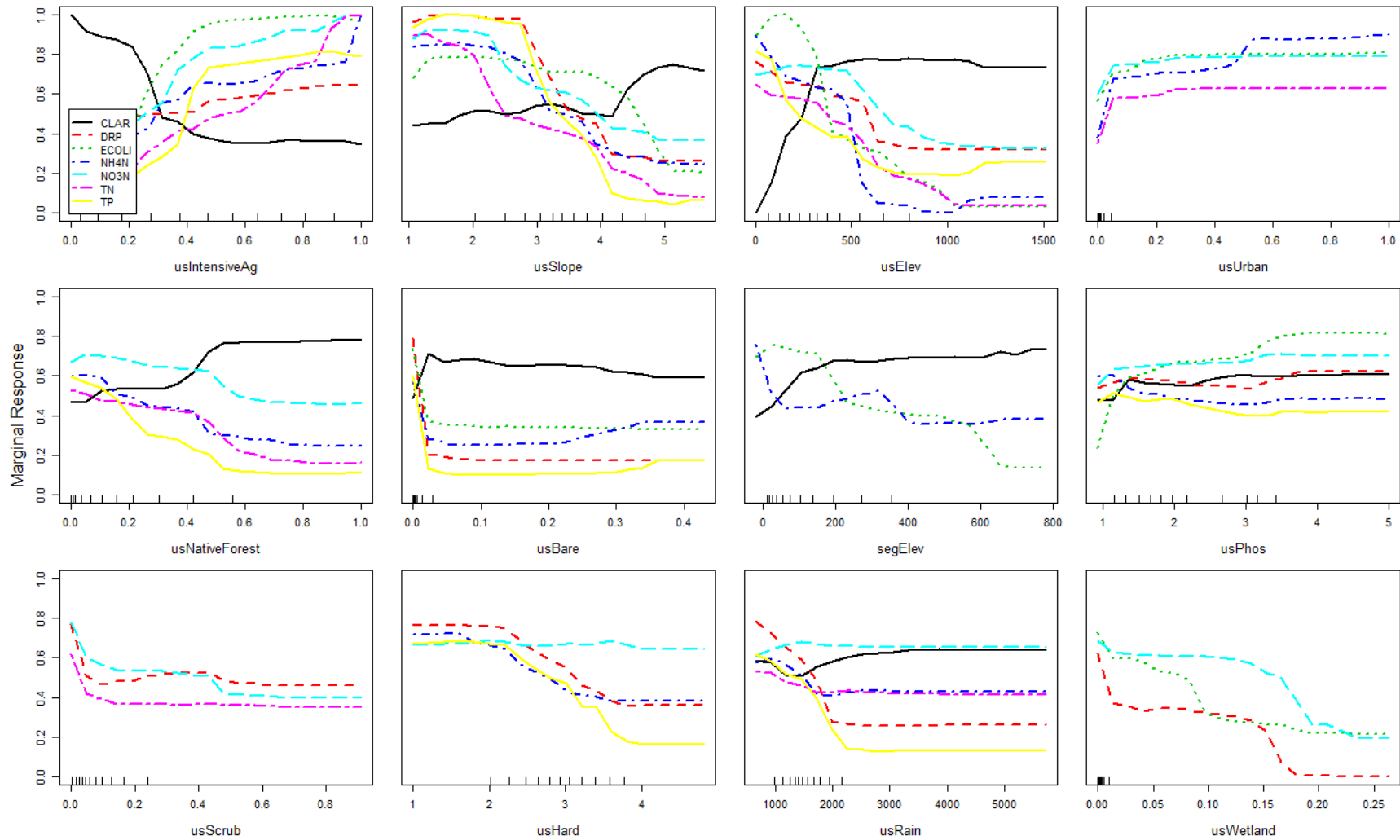


Figure 4-4: Partial plots for the 12 most important predictor variables in Random Forest models of water quality (See Fig. 4-5 for MCI plots). Each panel corresponds to one predictor. The Y-axis scales: standardised value of the marginal response for each of the eight modelled variables. In each case, the original marginal responses over all twelve predictors were standardised to have a range between zero and one. Plot amplitude (the range of the marginal response on the Y-axis) is directly related to a predictor variable’s importance; amplitude is large for predictor variables with high importance. Legend in top left panel applies to all panels.

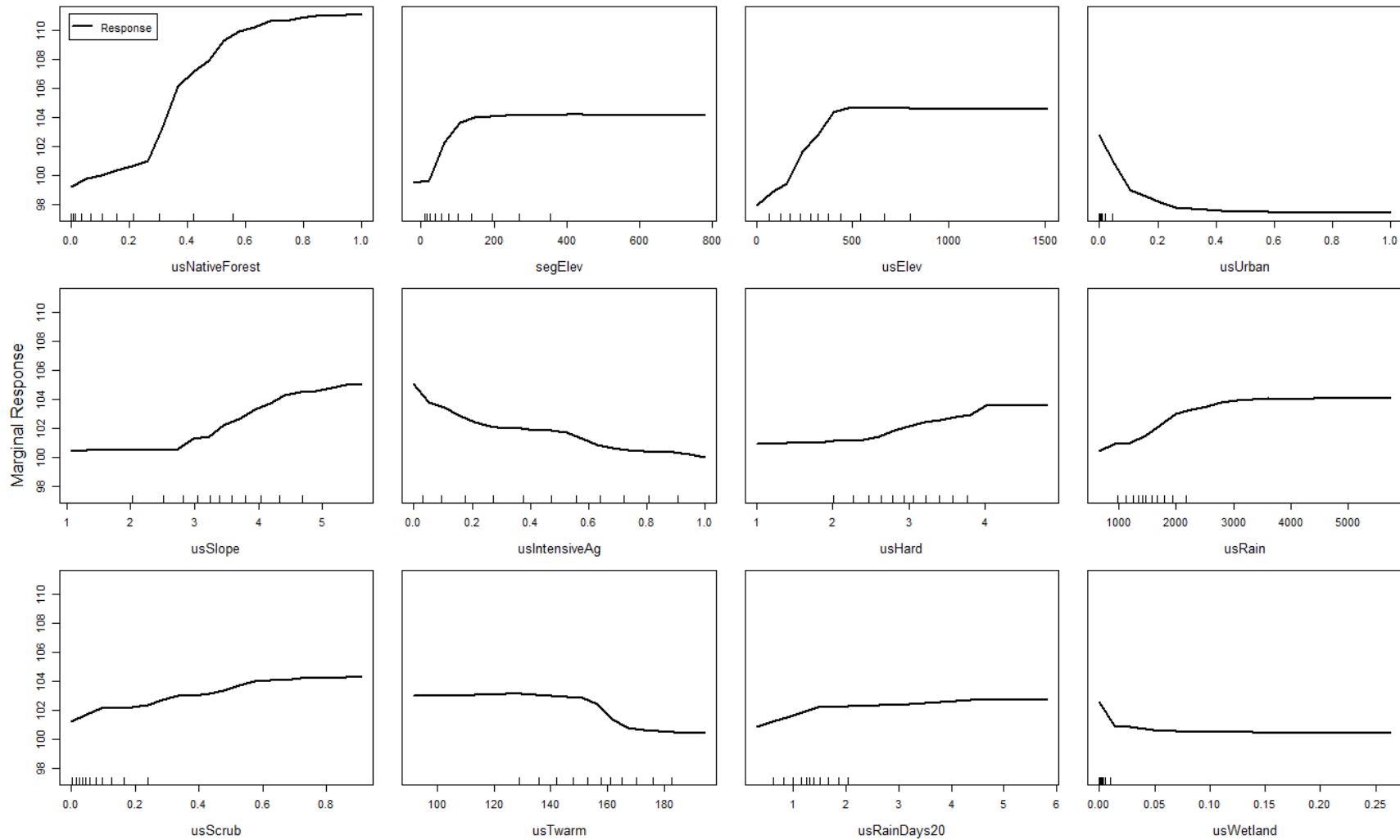


Figure 4-5: Partial plots for the 12 most important predictor variables for the MCI model. Each panel corresponds to one predictor variable. The Y-axis scale represents the absolute value of the marginal response (i.e. the scale represents the marginal change in MCI values). The amplitudes of the plots (i.e. the range of the marginal response shown on the y-axis) are directly related to a predictor variable's importance.

4.4 Model predictions

The minimum values predicted by the RF models were always somewhat larger than the minimum of the observed values and the maximum predicted values were always somewhat smaller than the maximum observed values (Table 4-3). This is an expected outcome of RF models, which are based on partitioning the data and predictions are derived from the means of observations that are assigned to a particular partition. As a consequence, the predictions for each water quality variable were always within the range of the observations.

Table 4-3: Comparisons of the minimum and maximum observed and predicted values of water quality variables.

Variable and unit	Minimum observed value	Maximum observed value	Minimum predicted value	Maximum observed value
CLAR (m)	0.1	12	0.3	9
DRP (mg/m ³)	0.5	290	1.0	148
ECOLI (cfu/100 ml)	1.0	2,300	2.4	1,471
NH4N (mg/m ³)	0.7	850	2.2	282
NO3N (mg/m ³)	0.6	13,500	4.4	12,292
TN (mg/m ³)	34.9	15,004	52.0	9,027
TP (mg/m ³)	2.0	410	4.5	245
MCI (unitless)	59.8	152	65.3	145

The mapped predictions for all five nutrient species (DRP, TP, NH4H, NO3N, TN) and ECOLI have similar coarse-scale spatial patterns, with relatively high values in low-elevation areas on the east coasts of the North and South Island, and in the inland Waikato, Wairarapa Valley, Rangitikei-Manawatu coastal plain, Taranaki Ring Plain, and Auckland Region (Figs 4-7, 4-7, 4-9, 4-11, 4-12, 4-13). In contrast, predicted nutrient and ECOLI concentrations are generally low in major mountain ranges (e.g. Southern Alps, Kahurangi, Kaimanawa, and Tararua Ranges), in large areas of the Department of Conservation estate (e.g. Fiordland, Westland, Te Urewera, Egmont, Whanganui and Tongariro National Parks), and in smaller, native forest-dominated areas of Northland and the Coromandel Peninsula.

The low elevation areas characterised by high nutrient and ECOLI concentrations coincide with land used for intensive agriculture and with most of New Zealand's urban centres. High-intensity agricultural and urban land currently account for 60% of the land area below 350 m elevation (Larned et al. 2016). Within these areas, there are some finer scaled differences in predicted water quality. The Canterbury Plains are characterised by high TN and NO3N concentrations, and intermediate TP and DRP concentrations, and the Waikato-Hauraki Plains area is characterised by high concentrations of both nitrogen and phosphorus.

Note that the maps in Figures 4-6 – 4-13 consist of NZSegments of Order 3 and above, and some extensive lowland areas are dominated by low order streams (e.g. eastern Auckland, Tauranga).

Steep coastal areas of the Marlborough Sounds, Fiordland, Coromandel and Banks Peninsulas and offshore islands are also dominated by low order streams. The predicted water quality in low order streams in these areas is not shown on the maps in Figures 4-6 – 4-13.

Predicted DRP and TP concentrations are elevated in rivers draining catchments dominated by Tertiary Mudstones (e.g. eastern Wairarapa, and the Aorangi, Puketoi and Ruahine Ranges), and in rivers draining catchments dominated by volcanic andesites, rhyolites and ignimbrites (e.g. central volcanic plateau), as indicated in Figures 4-7 and 4-13. Evidence for phosphorus enrichment due to chemical weathering in these areas comes from several studies of geochemistry and river and lake chemistry (Timperley, 1983; Close and Davies-Colley, 1990, Eden and Parfitt, 1992; McGroddy et al. 2008). In some catchments with phosphorus-rich parent rock, chemical weathering and fertilisers and other anthropogenic phosphorus are all sources of river DRP and TP.

Large-scale geographic patterns in predicted MCI scores and CLAR are generally the inverse of those for chemical and microbial water quality (Figs 4-6 and 4-10). Predicted CLAR is relatively high and predicted MCI scores correspond to the excellent and good ecological states (as set out in Stark and Maxted (2008)) in mountainous areas, the Department of Conservation estate, and other areas dominated by native forest land cover. Predicted CLAR decreases and MCI scores correspond to the fair and poor states in low-elevation alluvial plains and other areas dominated by intensive agriculture and urban land cover. Predicted MCI scores are also fair to poor in some rivers in areas dominated by exotic forest and low-intensity agriculture land cover, such as Central Otago, southwest Canterbury and the Rotorua Lakes-Lake Taupo area.

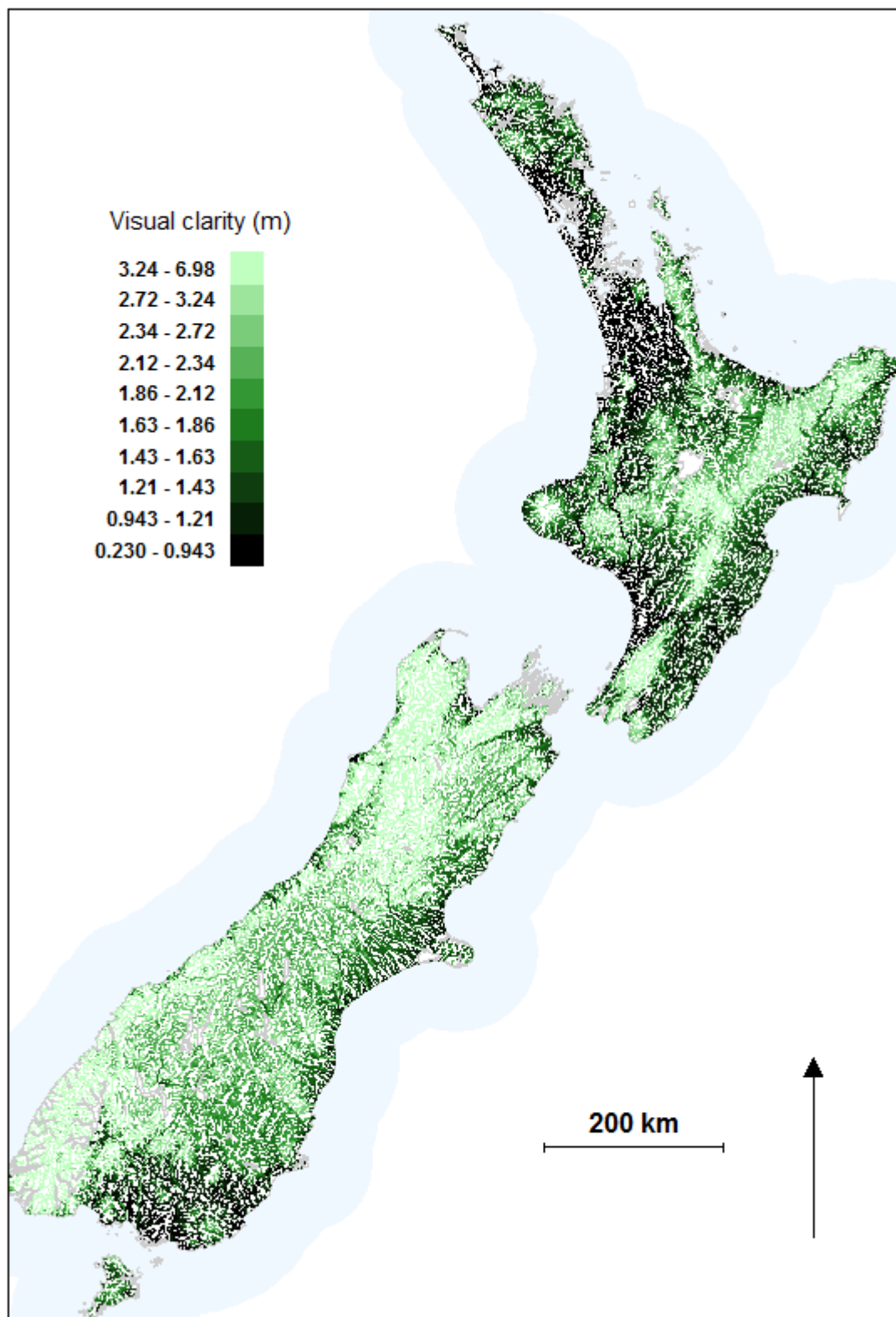


Figure 4-6: Predicted median visual clarity in New Zealand rivers. Map shows all NZSegments of Order 3 and higher. Smaller rivers are omitted to make river networks distinguishable.

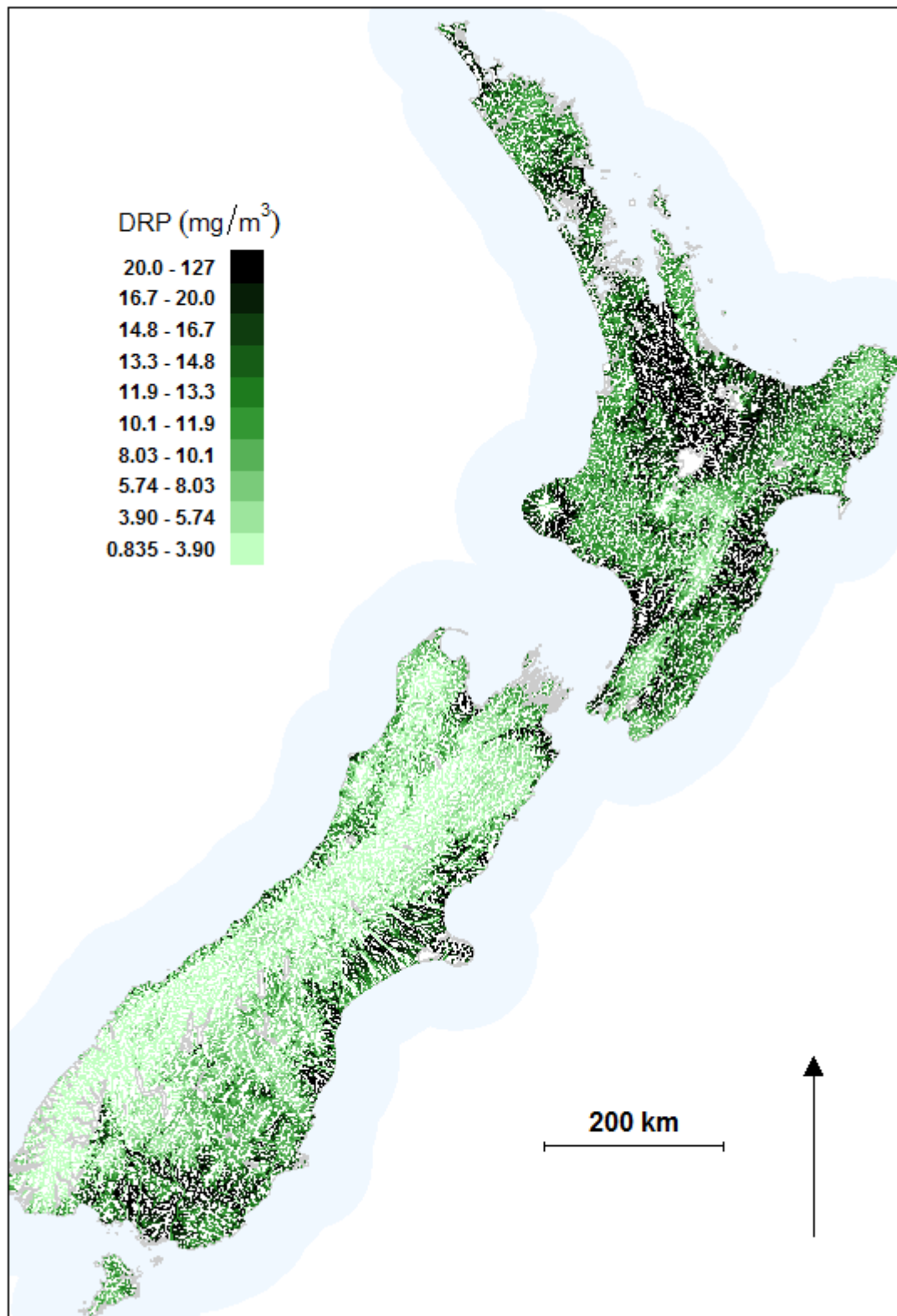


Figure 4-7: Predicted median DRP concentrations in New Zealand rivers of Order 3 and higher.

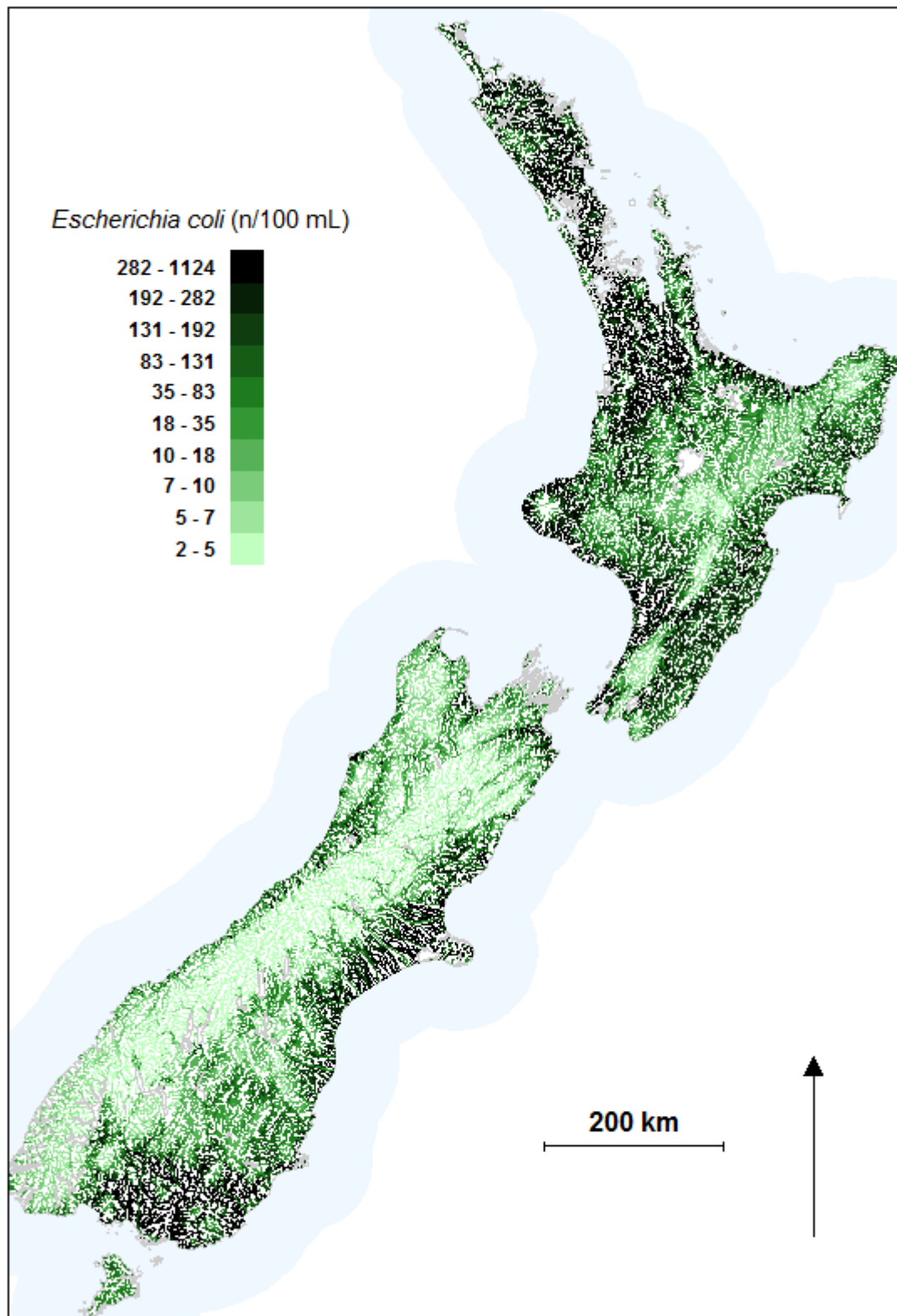


Figure 4-8: Predicted median *Escherichia coli* concentrations in New Zealand rivers of Order 3 and higher.

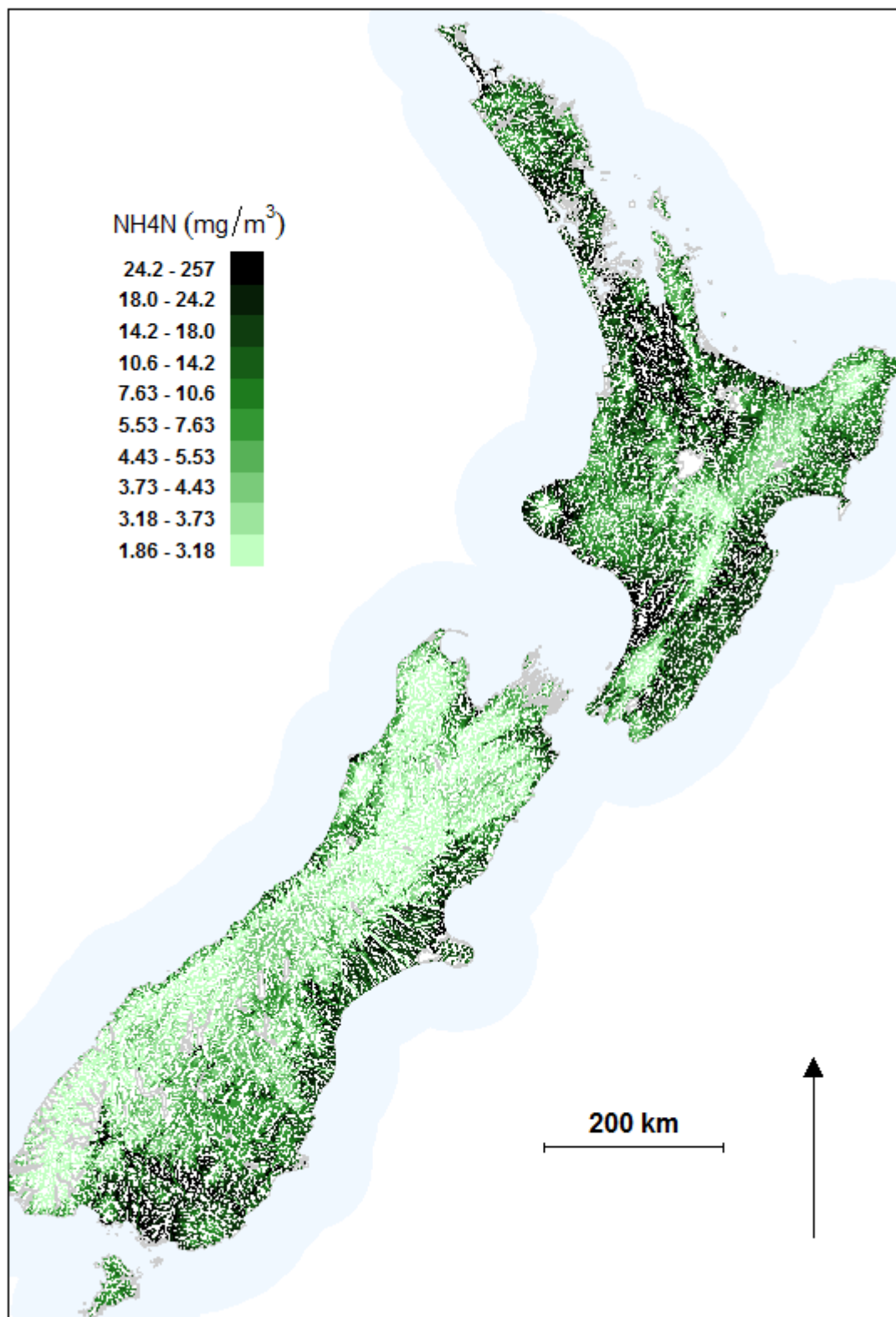


Figure 4-9: Predicted median NH₄N concentrations in New Zealand rivers of Order 3 and higher.

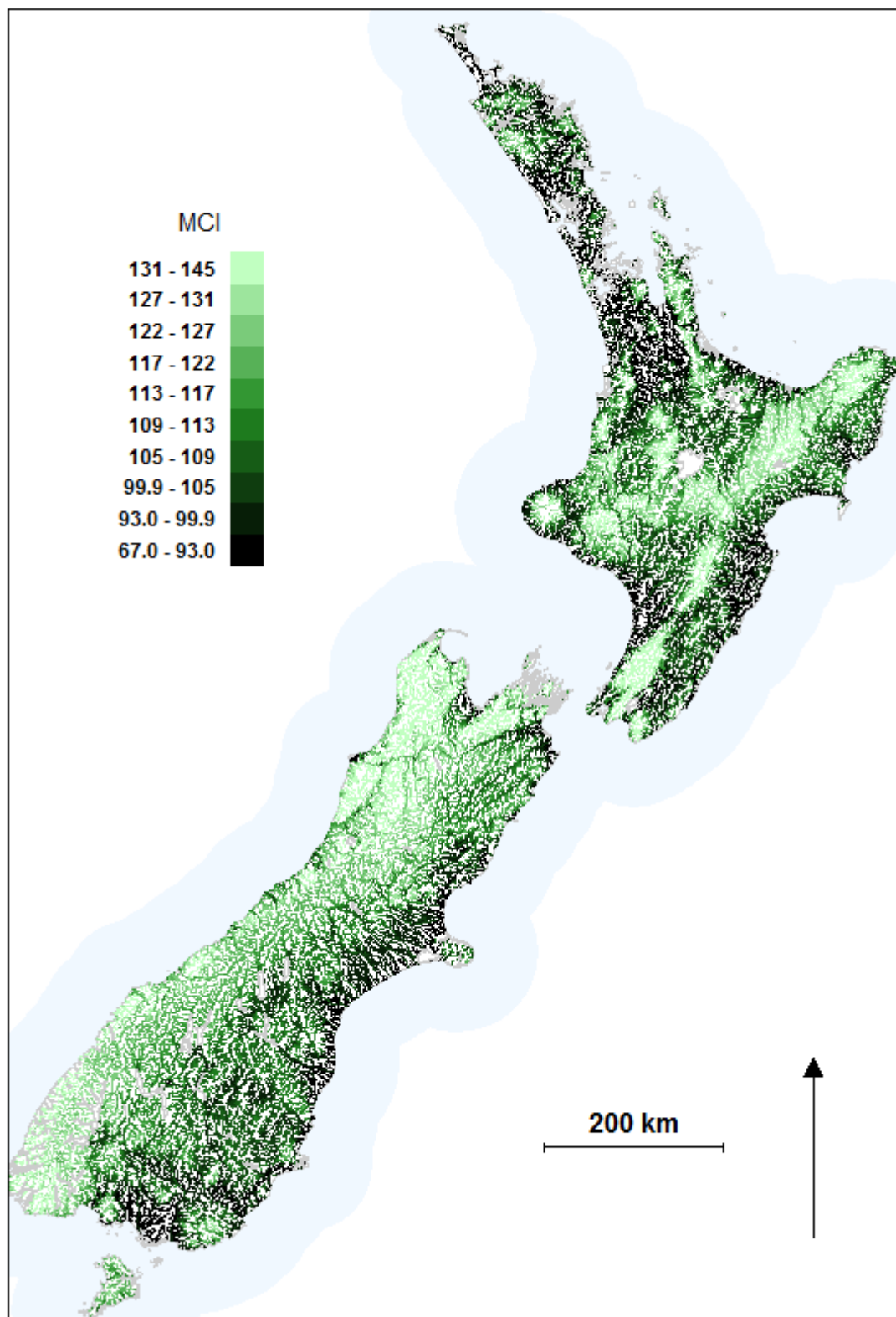


Figure 4-10: Predicted median MCI scores in New Zealand rivers of Order 3 and higher.

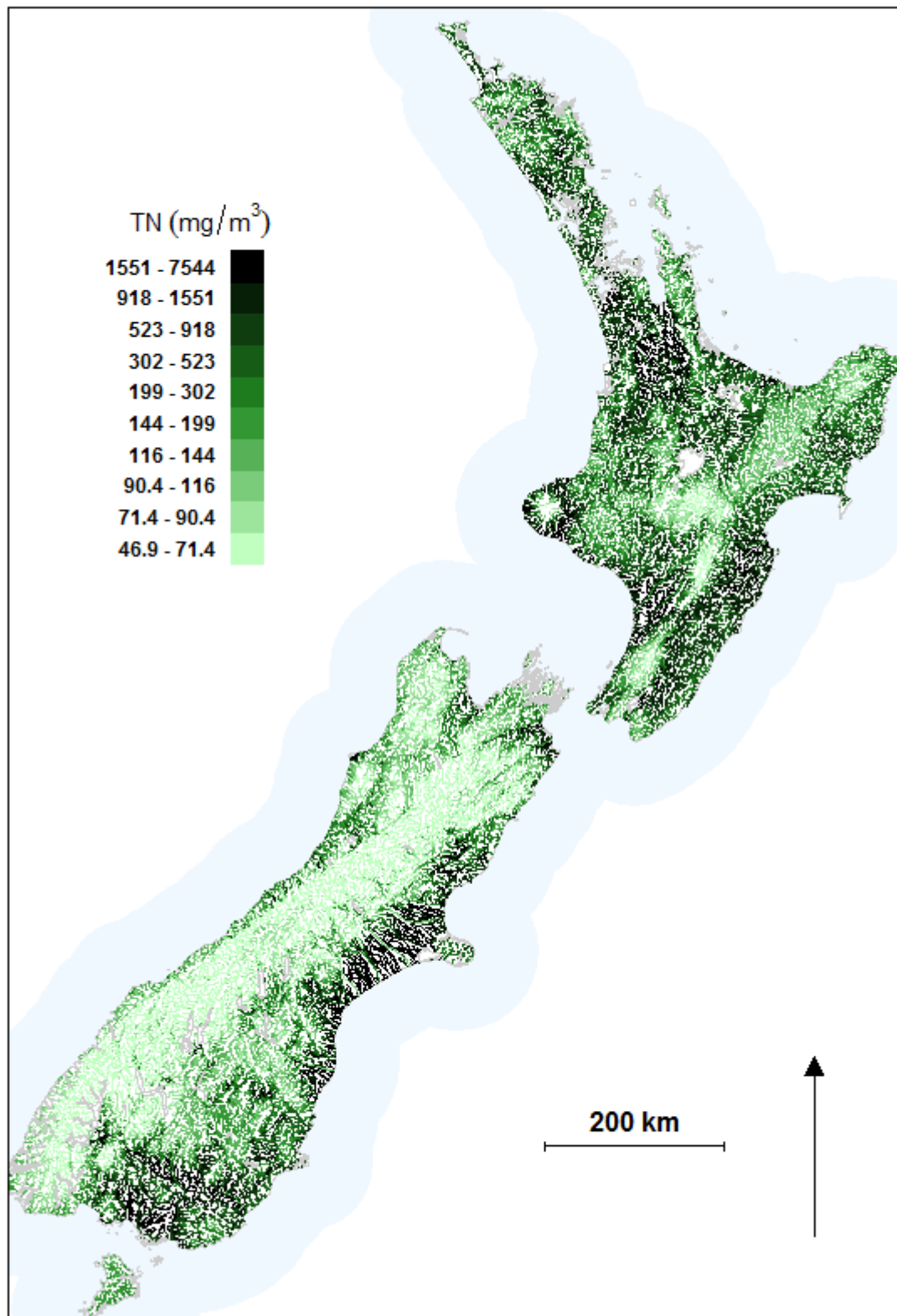


Figure 4-1: Predicted median TN concentrations in New Zealand rivers of Order 3 and higher.

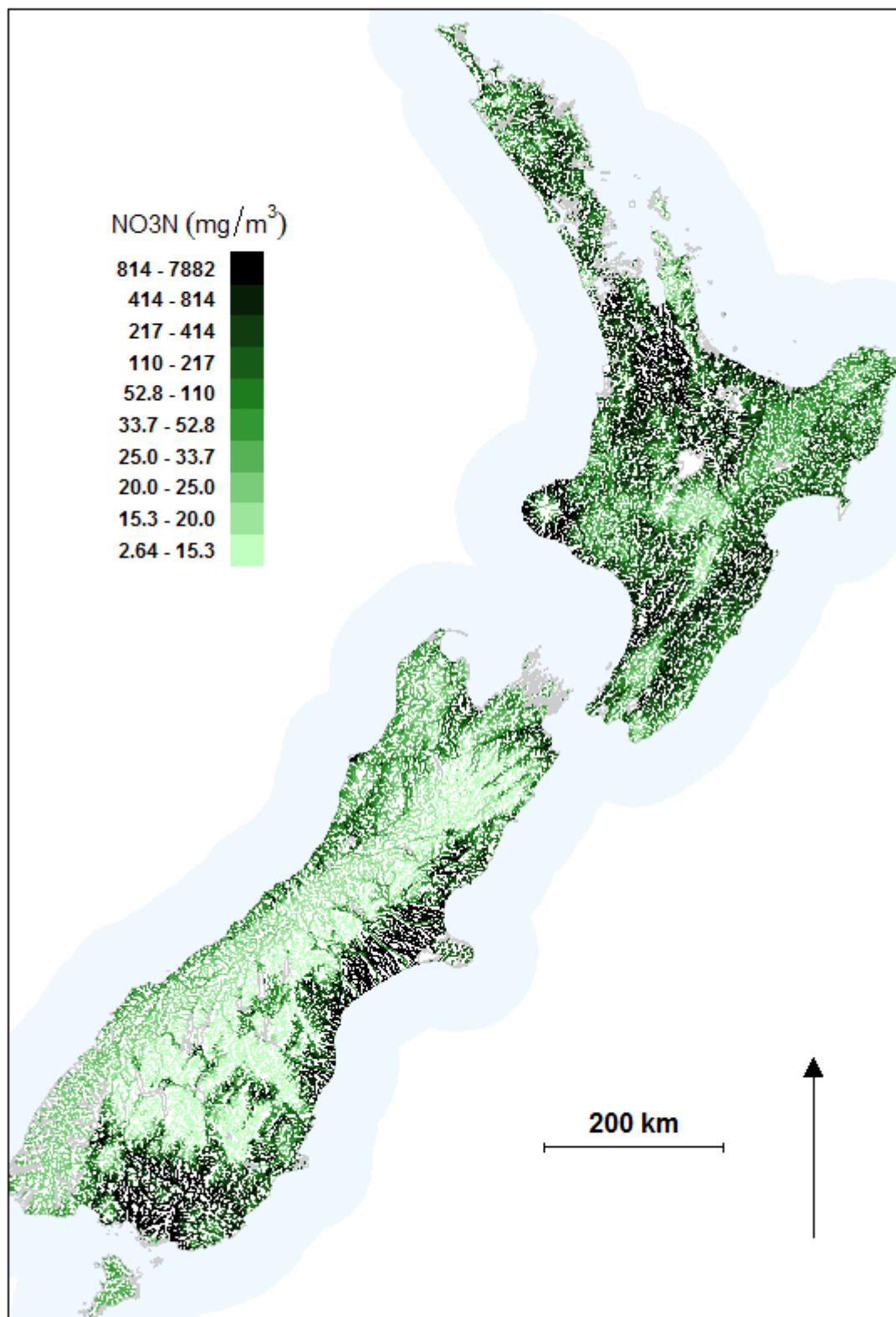


Figure 4-12: Predicted median NO₃N concentrations in New Zealand rivers of Order 3 and higher.

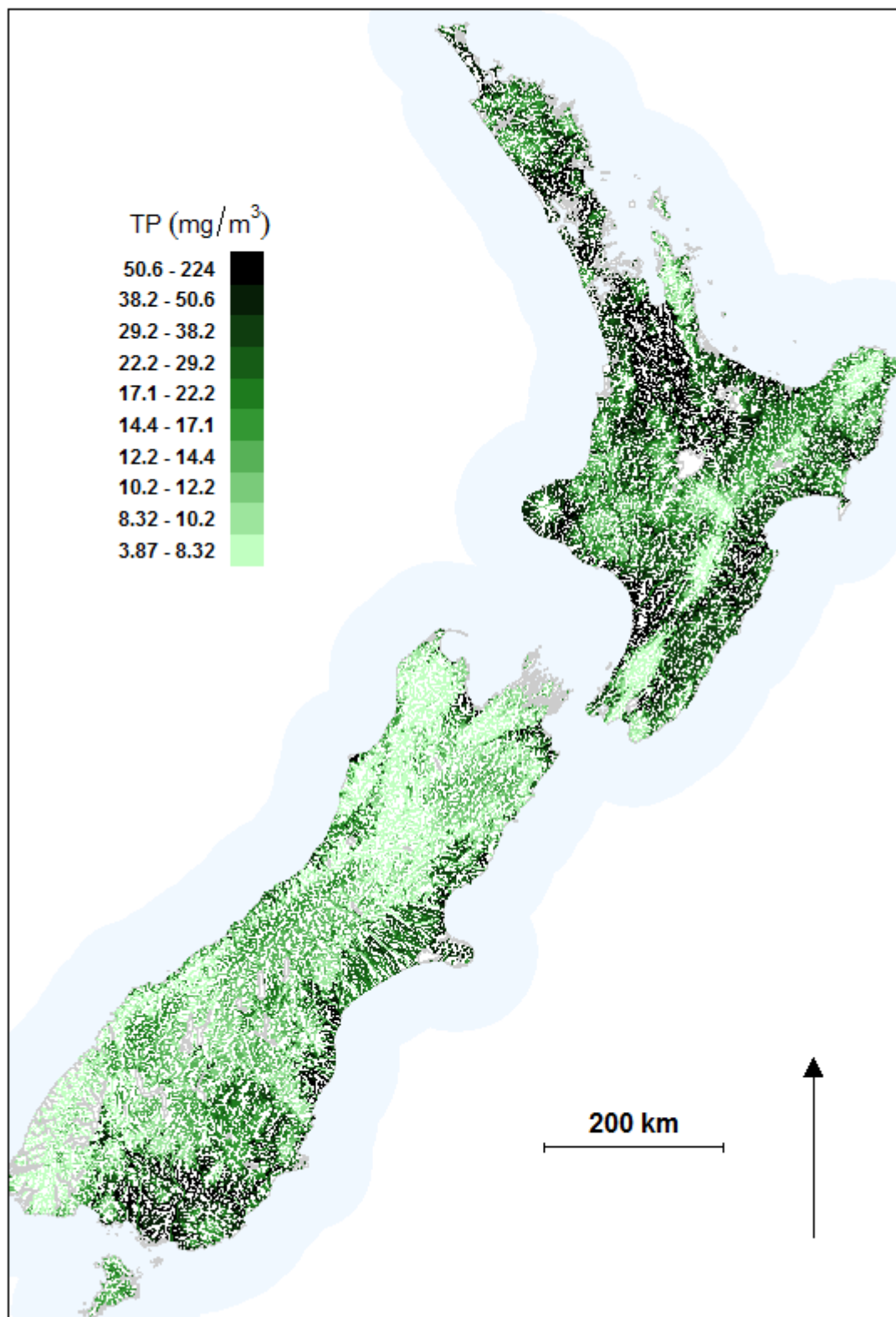


Figure 4-13: Predicted median TP concentrations in New Zealand rivers of Order 3 and higher.

5 Discussion

5.1 Comparison with previous studies

The river water quality models presented in this study update previous modelling work carried out by Unwin et al. (2010). The models in Unwin et al. (2010) were based on data for the period 1996-2007, and the models in the current study are based on data for the period 2009 to 2013. The results of the current study are generally consistent with those of Unwin et al. (2010) and the structures of the models (as indicated by the relative importance of predictor variables and directions of partial plots) are also similar. In addition, the performance of the models in the present study (as indicated by percent variance explained) was generally comparable to that of the Unwin et al. (2010) study.

The current study involved several improvements on the methodology used by Unwin et al. (2010). First, the current study used the recently updated REC2 digital network and associated attributes. Many of the updated attributes were used as predictor variables in the current study (e.g. hydrology variables, LCDB3 land cover). The updated digital network in the REC2 has a more accurate representation of rivers in many areas (e.g. low-gradient, low-elevation areas) than in the REC1.

The second difference was the use of (usIntensiveAg) as a predictor variable in the current study. This variable represents the combination of three LCDB3 land cover classes, High Producing Exotic Grassland, Short-rotation Cropland, and Orchard Vineyard & Other Perennial Crops. Unwin et al. (2010) used High Producing Exotic Grassland alone (which they referred to as %Pastoral Heavy). Our composite predictor usIntensiveAg follows recent work in which all intensive agricultural land cover classes were combined in a single variable to better reflect agricultural pressure on water quality outcomes (McDowell et al. 2012; Larned et al. 2016).

The third difference in the current study was the correction of model predictions for retransformation bias, following the method of Duan (1983). This was an omission in the original work of Unwin et al. (2010). With the exception of the MCI model, the RF model responses for water quality state are non-linear because the original values were \log_{10} -transformed. The predictions from these models are therefore subject to “retransformation bias”, which causes the back-transformed predictions to be under-estimated (Duan 1983). The correction factors we applied to the predictions (Equation 1) ranged from 1.13 - 1.72. Despite these correction factors, the maximum predicted values were always smaller than the maximum of the observed values (Table 4-3).

The fourth difference in the current study was the use of a stepwise predictor variable reduction process to eliminate redundant predictors from the RF models. No variable reduction was carried out in the Unwin et al. (2010) study. Elimination of redundant predictors does not alter the predictive performance of the RF models, but it helps with model interpretation by reducing the number of variables. The models in Unwin et al. (2010) had ≥ 28 or more predictor variables, whereas the models in the current study had ≤ 23 predictors, with a minimum of 11 (Table 4-2). Despite the reduction in predictor variables, many predictors in the current study made statistically significant contributions to predicted patterns of water quality at the national scale. The diversity of important predictor variables in the models reflects the fact that water quality is influenced by a complex mixture of natural and anthropogenic processes (e.g. geochemical reactions, atmospheric deposition, anthropogenic nutrient input, geomorphic processes, microbial activity).

In a previous study, Clapcott et al. (2013) fitted an RF model to site median MCI scores and reported a cross-validated R^2 of 0.63. Clapcott et al. (2013) also reported a cross-validated R^2 of 0.64 with an

alternative technique, boosted regression trees. The equivalent R^2 statistic for the MCI model in the current study was 0.69 (Table 4-1). The small improvement in performance in the current study may reflect the longer term dataset and the use of the REC2 river network.

5.2 Model uncertainty

In this study, we modelled broad scale patterns in water quality using catchment characteristics and segment scale descriptors as predictor variables. Because the processes determining water quality at any location are complex, some unexplained variation in our models is to be expected. Predictions made for individual locations are associated with uncertainties that are characterised by model RMSD (Table 4-1). However, the level of model bias for each water quality variable was low, which indicates that the predicted patterns reflect broad scale relative differences between locations.

The 95% confidence intervals for values predicted by our models for individual segments can be obtained using the following equations. Equation 1 should be used for calculating the intervals for the MCI predictions. Equation 2 should be used for calculating the intervals for the other water quality variables for which the variables were \log_{10} transformed prior to model fitting and the prediction uncertainty (RMSD) values have been reported in the \log_{10} transformed space.

$$95\% \text{ CI} = x \pm 1.96 \times \text{RMSD} \quad \text{Equation 1}$$

$$95\% \text{ CI} = 10^{[\log_{10}(x) \pm 1.96 \times \text{RMSD}]} \quad \text{Equation 2,}$$

where x is the estimated value in the original units, RMSD is the model error and 1.96 is the standard normal deviate or Z-score for probability ($0.025 \leq Z \leq 0.975$). The prediction confidence intervals for the \log_{10} -transformed variables, when expressed in the original units of the variables, are asymmetric and their values vary in proportion to the predicted water quality value. For example, if we let x be a predicted value for CLAR of 0.1 m, the lower and upper 95% confidence intervals are 0.04 and 0.25 m, respectively, whereas if x is 1.0 m the lower and upper 95% confidence intervals are 0.4 and 2.5 m, respectively.

RF model performance differed among water quality variables (Table 4-1). This variation may be attributable to differences in the biophysical processes that control those variables. Some biophysical processes may be poorly represented by our catchment-averaged spatial predictor variables. For example, concentrations of dissolved and total nitrogen and phosphorus in rivers are influenced to differing degrees by adsorption-desorption processes, deposition and suspension, and biological assimilation, transformation and removal; these mechanisms are not explicitly represented in the RF models. The absence of predictors that account for these and other processes means that some level of unexplained variation is inevitable.

5.3 Alternative modelling methods

The RF method that we used to develop river water quality models is well suited to data from monitoring sites that represent a wide range of environmental conditions. However, it is not the only method available. Alternative statistical models include generalised additive models (GAMs; Hastie et al. 2001), artificial neural networks (e.g. Joy and Death 2001), and boosted regression trees (e.g. Leathwick et al. 2005). We did not employ these alternatives, but it is possible that some water quality applications would be better served by models developed by one of the alternative methods. In particular, if it is important to identify areas with potentially extreme water quality values, models such as GAMS that can extrapolate beyond the range of the fitting data would be useful. In addition, models that incorporate biophysical processes (e.g. CLUES; Alexander et al. 2002) are available; in

some circumstances, process models are better suited to inform environmental policy. We considered RF models to be the best tool for predicting river water quality state for national scale reporting for 3 general reasons:

1. Spatial data that correspond to land cover and other environmental characteristics are widely available in New Zealand. These data are suitable for investigating associations between water quality and environmental characteristics, and empirical models are appropriate tools for identifying those associations. In contrast, process models require measurements or estimates of catchment processes (e.g. erosion, contaminant transport and transformation) and these data are in far shorter supply. In addition, process models are generally more time consuming and complex to calibrate than purely empirical models.
2. RF model predictions can be mapped at scales ranging from single network segments to the entire county. These maps provide a useful description of spatial patterns in water quality for environmental reporting purposes.
3. Among empirical modelling methods that generate associations between water quality and environmental characteristics, RF models have several advantages: they are minimally affected by multi-collinearity among predictor variables, they cannot be over-fitted, and they are unaffected by variation in data distributions. RF models cannot predict beyond the range of the observations, which may limit their utility in some applications. In the present study, limiting model predictions to the range of observations was a positive attribute as it ensured that those predictions were conservative.

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