Predicting Water Quality in the Great Barrier Reef Catchments: Learning from Long-Term Water Quality Monitoring Data

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Abstract

Riverine water quality deterioration has become a global issue, affecting freshwater and near-shore marine ecosystems. To protect aquatic environmental health in these systems, effective water quality management strategies are critically important. Riverine water quality needs to be evaluated and managed at the catchment scale. Management decisions can be greatly supported and informed by understanding of: (1) the processes influencing water quality constituent concentrations; and (2) the key factors affecting these processes and by predictive capability. As such, catchment water quality modelling tools are important to gain this knowledge and predict water quality dynamics under different climatic and land use scenarios.

A key challenge in modelling stream water quality dynamics is that there is the lack of comprehensive understanding of the role and importance of the various factors that drive differences in water quality across space and time, specifically: 1) the importance of catchment characteristics on the spatial variability in water quality; and 2) the importance of variations in environmental variables including weather and vegetation cover on the temporal variability in water quality in different landscapes. These issues have jointly led to a lack of predictive power of water quality models for multiple catchments over large regions.

This research aims to improve current understanding of how riverine water quality varies spatially and temporally and the factors that drive this and to develop improved data-oriented analytical and predictive frameworks to achieve this. In this research, I investigated long-term, multiple-site water quality monitoring datasets to identify the dominant factors affecting pollutant processes and thus to inform water quality management. This research focused on the Great Barrier Reef (GBR) catchments in sub-tropical and tropical north-eastern Australia. The GBR has high environmental, societal and economical values both nationally and globally. This thesis contains three results chapters to achieve the overarching research objective.

Chapter 4 addresses the spatial pattern of water quality and its linkage with heterogeneity in catchment landscape characteristics, using multivariate statistical analyses. By comparing spatial differences in long-term averaged water quality and

catchment landscape characteristics, two groups of catchments were identified. This grouping reflected the main differences in water quality: group one sites had lower time-averaged concentrations (except for NO_X), which were situated in wet areas with high sugar cane production and conservation zones, while group two sites had relatively higher average concentrations, were drier and with considerable grazing land use.

Chapter 5 reports on an investigation into the relationships between spatial variability in water quality and catchment characteristics, using a multi-model statistical modelling approach. Specifically, the aim was to identify key catchment characteristics influencing average event-mean concentrations and to develop a spatial model predicting this. Results indicated that natural catchment characteristics were important factors for determining the variation of sediments and particulate nutrients over space, while anthropogenic characteristics (i.e., land use) were more important factors for dissolved nutrients species. The models developed were able to predict average event-mean concentrations well, with Nash-Sutcliffe efficiency (NSE) ranging from 0.64 to 0.98.

Chapter 6 presents an investigation into the key factors affecting temporal changes in water quality, as summarized by variations in constituent event-mean concentrations. A Bayesian hierarchical modelling coupled with a Bayesian model averaging approach was used to evaluate the temporal change in stream water quality. The modelling results demonstrated that the key temporal controls varied between the two clusters of sites identified in Chapter 4, as well as among different constituents. Overall, catchment ground cover condition and soil moisture prior to runoff events were of greatest importance in determining the temporal change in event-mean concentration and event discharge characteristics were also important.

Results from the three chapters were brought together to assess the degree to which the result has the potential to support the current water quality management and inform future design of water quality management in the GBR catchments. The spatial modelling results support the current working hypotheses underpinning water quality management in the GBR catchments, that cattle grazing, and sugarcane land uses are management priorities to reduce sediment and dissolved

inorganic nitrogen, respectively. Based on the temporal modelling results, the future management practices could focus on maintaining good vegetation cover, especially for large and grazed catchments before the wet season. Finally, the water quality modelling framework used in this research provides a potential tool to evaluate catchment water quality, and what can be done to improve it, under future changes to climate, land uses and land management.

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Declaration

This is to certify that:

i. This thesis is an original work of the author alone except where due acknowledgement has been made.
ii. The work has not been submitted previously, in whole or in part, to qualify for any other degree or qualification in any other universities.
iii. The content of the thesis is the outcome of the research which has been carried out during the official PhD candidature.
iv. The thesis contains less than 100,000 words in length, exclusive of tables, maps, bibliographies and supplementary materials.

Shuci Liu

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Preface

This thesis is framed within the Australian Research Council (ARC) Linkage Project (LP140100495) – Predicting water quality at the catchment scale: learning from two decades of monitoring, funded by the Australian Research Council, the Queensland Natural Resources, Mines and Energy, the Environment Protection Authority Victoria, the Department Land for Environment Water and Planning Victoria and the Australian Bureau of Meteorology. The project addressed water quality across the state of Victoria and in the Great Barrier Reef catchments, northeast Queensland, Australia. This thesis focuses on the Great Barrier Reef catchments. This thesis presents research that has been conducted during my PhD candidature, from 2016 to 2019, at the Department of Infrastructure Engineering, The University of Melbourne. Water quality data used in this research were provided by the Queensland Department of Environment and Science. This thesis only includes the original works to achieve this PhD degree, with no material being submitted for another qualification. In addition, Chapters 4 to 6 are each formatted as a research article that has been either published or submitted for possible publication as follows:

- Chapter 4 has been published as Liu, S., Ryu, D., Webb, J., Lintern, A., Waters, D., Guo, D., & Western, A. (2018). Characterisation of spatial variability in water quality in the Great Barrier Reef catchments using multivariate statistical analysis. Marine Pollution Bulletin, 137, 137-151. https://doi.org/10.1016/j.marpolbul.2018.10.019.
- Chapter 5 has been submitted as Liu, S., Ryu, D., Webb, J., Lintern, A., Waters, D., Guo, D., & Western, A. Understanding the impacts of catchment characteristics on spatial variability in water quality: a case study in the Great Barrier Reef catchments. Submitted to Water Resources Research, and currently in revision.
- Chapter 6 will be submitted as Liu, S., Ryu, D., Webb, J., Lintern, A., Waters, D., Guo, D., & Western, A. (2019). Key factors influencing temporal variability in stream water quality in the Great Barrier Reef

catchments. Will be submitted to Water Resources Research, and currently under internal review.

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Abbreviations

Abbreviations	**Description**
AET	Actual evapotranspiration
ANN	Artificial neural networks
APHA	American Public Health Association
APSIM	Agricultural production systems simulator
APVMA	Australian Pesticides and Veterinary Medicines Authority
AWAP	Australia water availability project
AWRA	Australia water resources assessment
BHM	Bayesian hierarchical modelling
BMA	Bayesian model averaging
BMP	Best management practice
BOD	Biochemical oxygen demand
BoM	Bureau of Meteorology, Australia Government
CA	Cluster analysis
COTS	Crown-of-thorns starfish
CTF	Controlled traffic farming
CV	Coefficient of variation
DAF	Department of Agriculture and Fisheries, Queensland Government
DELWP	Department of Environment, Land, Water and Planning, Victoria Government
DES	Department of Environment and Science, Queensland Government
DIC	Dissolved inorganic carbon
DIN	Dissolved inorganic nitrogen
DN	Denitrification process
DNRME	Department of Natural Resources, Mines and Energy, Queensland Government
DO	Dissolved oxygen
DOC	Dissolved organic carbon
DON	Dissolved organic nitrogen
DOP	Dissolved organic phosphorus
EC	Electrical conductivity
EMC	Event mean concentration
EU	European Union
EVI	Enhanced vegetation index
FA	Factor analysis
FMA	Frequentist model averaging

FRP	Filterable reactive phosphorus
GAM	Generalised additive modelling
GBR	Great Barrier Reef
GBRCLMP	Great Barrier Reef Catchment Loads Monitoring Program
GCMs	Global climate models
GLMM	Generalized linear mixed model
GVS	Gibbs variable selection
HRU	Hydrologic response unit
HSPF	Hydrologic simulation program-Fortran
IWRM	Integrated water resources management
LOD	Limits of detection
LUCC	Land use/land-cover change
MCMC	Markov chain Monte Carlo
MODIS	Moderate resolution imaging spectroradiometer
NDVI	Normalised difference vegetation index
NH_4	Ammonium nitrogen
NI	Nitrification process
NO_X	Oxidised nitrogen
NRM	Natural resource management
NSE	Nash-Sutcliffe efficiency
OLS	Ordinary least square
PCA	Principal component analysis
PN	Particulate nitrogen
POC	Particulate organic carbon
PP	Particulate phosphorus
PSII	Photosystem II inhibiting herbicide
R^2	Coefficient of determination
RF	Random forests
SPV	Subjects per variable
SWAT	Soil water assessment tool
TMDL	Total maximum daily load
TN	Total nitrogen
TP	Total phosphorus
TSS	Total suspended solid
WMIP	Water monitoring information portal
USGS	United States Geological Survey

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Chapter 1 Introduction

1.1 Background

1.1.1 Degradation in coral cover in the Great Barrier Reef

In the last century, the world's coral reefs have suffered from considerable degradation in many marine ecosystems (Bellwood et al., 2019). In Australia, coral cover in the Great Barrier Reef (GBR) has decreased significantly (Bridge et al., 2019; Brodie et al., 2013c; Hughes et al., 2017; Puotinen et al., 2016). In the northern GBR, it has been estimated that about half of the coral cover experienced bleaching in 2016-2017 (Oliver et al., 2018; Ortiz et al., 2018). Coral decline was found to be caused by a range of threats, among which, water quality degradation is one of the most important (Brodie et al., 2012; Hunter & Walton, 2008; McKergow et al., 2005b). The GBR marine ecosystem has experienced significant water quality deterioration, mainly due to agricultural intensification and urban settlement in the adjacent catchments (Carroll et al., 2012; Packett et al., 2009). These intensive activities have contributed to increased land-derived sediments, nutrients and pesticides polluting the waterways and GBR lagoon (De'ath & Fabricius, 2008; DeVantier et al., 2006).

Agricultural non-point source pollutants including fine sediments, nutrients and pesticides have detrimental effects on ecosystems in the GBR lagoon (Brodie et al., 2013a; Furnas, 2003; Packett et al., 2009; Thorburn et al., 2013). Nutrients pose high water quality risk to the GBR and have been closely linked to the outbreaks of crown-of-thorns starfish (COTS). COTS has been one of the most significant factors leading to the decline in coral cover (Hall et al., 2017; Haywood et al., 2019; MacNeil et al., 2019; Thorburn et al., 2013). Excessive nutrients and high turbidity also increased the chance of coral bleaching (Brown, 1997; Hoegh-Guldberg, 1999; Wiedenmann et al., 2013; Zaneveld et al., 2016). Fine sediments derived from soil erosion have resulted in a reduction in the light penetration that is essential for marine ecosystems, including for seagrass and coral reefs (Brodie et al., 2013c; McCulloch et al., 2003; Wolanski et al., 2005). Extensive pesticides application to crops has also had negative impacts on freshwater and inshore coastal habitats (Brodie et al., 2017b; Lewis et al., 2014; Richmond et al., 2018).

1.1.2 Drivers of reduced water quality

Water quality in streams is highly variable in space and time, with many influencing factors due to processes such as pollutant generation and transport (Haynes et al., 2007; Tong & Chen, 2002). A better understanding of the environmental drivers of water quality could potentially inform land management practices that aim to reduce the flux of pollutants (Butler et al., 2013). Spatial heterogeneity in catchment landscapes and temporal changes in environmental conditions (e.g. hydroclimate and ground cover) have led to high spatial and temporal variability in water quality between and within catchments (Botter et al., 2019; Lintern et al., 2018a; Shi et al., 2019). However, the controls on water quality dynamics at the catchment scale are poorly understood, with spatial and temporal water quality drivers typically investigated in isolation. For example, whilst there have been a large number of studies that have assessed the impact of land use on spatial differences in water quality (Ahearn et al., 2005; Carlson et al., 2019; Dillon & Kirchner, 1975), few studies have addressed the impact of land use on the relationship between hydroclimatic parameters and water quality (e.g., discharge-concentration relationships) (Bieroza et al., 2018).

1.1.3 Monitoring of surface water quality

To report on the status of fresh and coastal waters, regional water quality monitoring and modelling programs have been developed around the world (Strobl & Robillard, 2008). For example, under the European Union (EU) Water Framework Directive, each member state has implemented water quality monitoring programs to improve both water quality and ecological health, and to provide evidence the effects for land management actions (Skeffington et al., 2015; Voulvoulis et al., 2017). Additionally, the United States Geological Survey's National Water-Quality Assessment (NAWQA) was implemented in 1991, providing scientific data and knowledge on the quality of river, groundwater, and aquatic ecosystems at different scales (e.g., state and national) (Read et al., 2017; USGS, 2019). It remains challenging to learn from multi-constituent and multi-site water quality monitoring data because of the complexity within the processes of water quality dynamics. Interpretation of these water quality monitoring data is important to support management decision-making.

1.1.4 Modelling of surface water quality

Water quality modelling is one way to improve our understanding of water quality dynamics. As the implementation of more long-term water quality monitoring programs over the past few decades, catchment modelling tools have been developed (Abbaspour et al., 2015; Rauch et al., 1998; Taylor et al., 2016; Tchobanoglous & Schroeder, 1985). Although these modelling tools have advanced the understanding of water quality dynamics, they remain inadequate either for representing multiple sites (Godsey et al., 2009), or the direct interpretation of water quality monitoring data (Arnold & Fohrer, 2005; Carr & Podger, 2012). This is due to the limitations in water quality assessment tools (e.g., modelling techniques).

1.2 Research Objectives

A robust and rigorous monitoring and modelling framework that can simultaneously assess and model temporal trends in water quality over multiple catchments is required to understand and predict both the between-site and within-site variability in water quality. In the GBR catchments, there has been more than a decade of both monitoring and modelling water quality (Smith et al., 2012). The Paddock to Reef Integrated Monitoring, Modelling and Reporting Program, together with Great Barrier Reef Catchment Loads Monitoring Program have collected water quality data over the last decade (Huggins et al., 2018; Shaw & Silburn, 2014). This program has provided an opportunity to interpret monitoring data through a data-oriented modelling tools that can advance our understanding of the interactions between water quality and human activities or natural catchment processes.

This thesis focuses on enhancing our understanding of the key controls on water quality in the GBR catchments over space and time, and ultimately informing the development of future catchment management strategies. The broad research objectives are: 1) to better understand the key controls on spatial and temporal variability in stream water quality in the GBR catchments; and 2) to develop a data-driven modelling framework for predicting water quality dynamics and performing future water quality assessment in the GBR catchments.

1.3 Thesis Structure

This thesis is structured as follows. Chapter 2 reviews relevant literature on the current status of stream water quality around the world, as well as in the GBR catchments and on commonly used water quality modelling approaches. At the end of Chapter 2, research gaps are identified, and the research questions are stated. Chapter 3 describes the overarching conceptual framework of this research and provides an introduction of the study area and data sets used. Chapters 4 to 6 present the key analyses undertaken and their interpretation. Each of these chapters has been formulated as a stand-alone research article (described in the preface). Each addresses a specific research question (Section 3.2). Finally, Chapter 7 discusses the strengths and limitations of this thesis, proposes future research directions, and summarizes the key contributions and conclusions of this thesis.

Chapter 2 Literature Review and Research Questions

2.1 Overview

This chapter aims to review the literature focusing on the water quality in general, as well as in the context of the Great Barrier Reef. This literature review starts with a broader review of the current knowledge of the potential factors affecting spatial and temporal variations in riverine water quality (Section 2.2). Section 2.3 summaries the causes of significant degradation of coastal and marine ecosystems, and the key groups of constituents that impact the marine ecosystems. Then, a summary of available catchment water modelling techniques is introduced in Section 2.4. The chapter concludes with a summary of the key knowledge gaps, and the corresponding research questions (Section 2.5) to address these gaps.

2.2 Factors Affecting Spatial and Temporal Variability in Stream Water Quality

The spatial and temporal dynamics of water quality in riverine systems are a result of complex interactions between pollutant processes in catchments (Chen et al., 2016b; Davis et al., 2017; Lintern et al., 2018a; Liu et al., 2018; Vrebos et al., 2017; Xu et al., 2019b). Understanding of the underlying processes that drive these variations is important to maintain the catchment ecosystems and make effective water resources management strategies (Dupas et al., 2019; Mohtar et al., 2019; Pionke et al., 2000; Sidle et al., 2006; Tim & Jolly, 1994).

Generally, spatial and temporal variation in water quality are driven by three key processes in catchments: 1) sources – the amount of pollutants available within a catchment; 2) mobilisation – detachment of pollutants from the source by processes such as erosion and weathering; and 3) delivery – the transport of the detached pollutants to the receiving waters via surface or subsurface flow (Granger et al., 2010). From a more detailed process perspective, processes can be classified into three key groups: atmospheric deposition, hydrologic and geomorphic processes;

biogeochemical processes (e.g., nutrient cycling); and the impacts of alternative land management (Islam et al., 2001; McNamara et al., 2006). Overall, the source, mobilisation and delivery of the pollutants varies both spatially and temporally, resulting in spatial and temporal changes in water quality constituent concentrations. The existing literature (Table 2-1) indicates that heterogeneity in catchment landscape characteristics is linked to the spatial difference in water quality across different catchments, while hydroclimatic and vegetation dynamics are more relevant to temporal variation in constituent concentration within a catchment (Bartley et al., 2012; Lintern et al., 2018a; Mellander et al., 2015; Merz, 2013; Onderka et al., 2012; Sharpley et al., 2002).

Table 2-1. Examples from the literature of demonstrated impacts of catchment spatial landscape characteristics and temporal varying environmental conditions on constituent source, mobilisation and delivery.

Potential factors	Process			Literature
	Source	Mobilisation	Delivery	
Spatial variation in water quality				
Land cover	✓		✓	Carroll et al. (2000), Li et al. (2009), Pratt and Chang (2012), Schilling et al. (2008), Wear et al. (1998), Larned et al. (2004)
Land use	✓	✓	✓	Dillon and Kirchner (1975), Heathwaite et al. (1990), Yellowlees (1990), Pekárová and Pekár (1996), Walling (1999), Tong and Chen (2002), Buck et al. (2004), Baker (2006), Kang et al. (2010), Wan et al. (2014a), Hu et al. (2019), Carlson et al. (2019)
Atmospheric deposition	✓	✓		Cosby et al. (1985), Riggan et al. (1994), Smith et al. (1997), Paerl et al. (2002)
Geology/soil type	✓	✓	✓	Dillon and Kirchner (1975), Quinn and Stroud (2002), Rothwell et al. (2010), Yang and Jin (2010), Varanka et al. (2015), Hounslow (2018).
Climate	✓	✓	✓	Smith et al. (1997), Hanrahan et al. (2003), Morrill et al. (2005),

				Kleinman et al. (2006), Pratt and Chang (2012), Green et al. (2014) ,Yan et al. (2015)
Topography		✓	✓	Kratz et al. (1997), Ekholm et al. (2000), Creed and Beall (2009)
Hydrology			✓	Kleinman et al. (2006), Hrachowitz et al. (2016)
Temporal variation in water quality				
Discharge	✓	✓	✓	Allan et al. (1997b), Evans and Davies (1998), Haygarth et al. (2004), Godsey et al. (2009), (Herndon et al., 2015), Bieroza et al. (2018), Zhang (2018), Zimmer et al. (2019), Chen and Chang (2019)
Soil water content	✓	✓	✓	Swank et al. (2001), Varanou et al. (2002), Clinton and Vose (2006), Sebestyen et al. (2008), Neary et al. (2009), Kincaid and Findlay (2009), Jencso et al. (2010)
Rainfall	✓	✓		Grayson et al. (1997), Schulz (2001), Neal et al. (2003), Kirchner et al. (2004), Prathumratana et al. (2008), Delpla et al. (2009), Park et al. (2011), Delpla et al. (2011)
Temperature	✓	✓		Cosby et al. (1985), Osborne and Kovacic (1993), Smith et al. (1997), Norton and Fisher (2000), Ducharne (2007), Varol and Şen (2009)
Ground cover	✓	✓	✓	Dabney et al. (2001), Buck et al. (2004), Ahearn et al. (2005), Li et al. (2008), Sahu and Gu (2009), Dosskey et al. (2010),

2.2.1 Spatial variability in water quality

Riverine water quality can vary markedly between catchments (Baker, 2006; Ekholm et al., 2000). Natural and anthropogenic characteristics of a catchment can influence the three key catchment processes, and thus lead to large spatial variation in water quality (Lintern et al., 2018a; Shi et al., 2019).

2.2.1.1 Anthropogenic landscape characteristics

Land use has been widely acknowledged as one of the key factors that can cause spatial variation in water quality (Aronson et al., 2014; Bramley & Roth, 2002; Calijuri et al., 2015; Hunter & Walton, 2008; Jiang et al., 2015; Lintern et al., 2018a; Nash & Chaloud, 2011). Land use can reflect the extent of non-point source pollution. For instance, land clearing and any associated intensification of agricultural activities post-clearing can result in an increase in nutrient loads from fertiliser application (Fraser et al., 2017; Reside et al., 2017). The generation of suspended sediments can also be caused by altering the surface soil properties (e.g., tillage) (Blevins et al., 2018; Muscutt et al., 1993; Skaggs et al., 1994; Stonestrom et al., 2009). For instance, there was a strong positive relationship between urban land use and annual average ammonium nitrogen (NH_4) (Guo et al., 2010a; Huang et al., 2013). In Australian streams, average event-mean concentrations of sediment and total phosphorus from dryland cropping dominated catchments can be 32 and 4 times greater, respectively, than those of natural forested catchments (Bartley et al., 2012).

Land use can also influence mobilisation and delivery processes. Variation in human activities across space can lead to different mobilisation and delivery patterns across catchments. Elevated mobilisation of sediments has been observed at locations with higher soil erosion potential, caused by, for example: 1) livestock activities (Carman et al., 2000; Herbst et al., 2012; Strand & Merritt, 1999); 2) gully formation on agricultural land (Gordon et al., 2008; Poesen et al., 2003; Poesen et al., 1996), and 3) long-term crop cultivation (Poesen et al., 1996; Skaggs et al., 1994). These activities also increase the mobilisation of particulate nutrients (e.g., PN and PP) (Bowes et al., 2015). In addition, land use can also affect constituent delivery. For instance, increases in agricultural and urban land use can result in a greater delivery rate of sediments and nutrients to the receiving waters (Heathwaite et al., 1990; Walling, 1999; Zhou et al., 2019). This is due to an extended drainage network with a greater hydrological connectivity (Stieglitz et al., 2003; Tockner et al., 1999). Rapid urbanization has also resulted in an increase in the amount of impervious surfaces (e.g., parking space and road), which linked to degradation through an increased pollutant load carried by the stormwater and severely altered hydrology (Bannerman et al., 1993; Brabec et al., 2002).

2.2.1.2 Natural landscape characteristics

The natural conditions of catchments (climate, hydrology, land vegetation cover, geology and topography) have an impact on the spatial variation in water quality (Dillon & Kirchner, 1975; Donohue et al., 2006; Lintern et al., 2018b; Singh et al., 2004; Ye et al., 2009). For instance, catchment geology and soil type determine the source of sediment and naturally-derived nutrients in catchments (Grayson et al., 1997; Holloway et al., 1998; Ice & Binkley, 2003). Catchments with higher sedimentary and igneous deposits have higher export of dissolved nutrients (Dillon & Kirchner, 1975). Additionally, higher salt levels have been detected in catchments with easily weathered bedrock (e.g. limestone) (Herczeg et al., 2001). Catchment geology also influences the mobilisation of sediment and particulate constituents (Kleinman et al., 2011; Lewis et al., 2013). For example, soil erodibility of the parent material was positively correlated with sediment export (Bakker et al., 2008; Beusen et al., 2005). Moreover, it has been shown that catchment topography can control water residence time at the catchment scale (McGuire et al., 2005), affecting time-dependent biogeochemical reactions for constituents such as nitrate (NO_3) (Hornberger et al., 2001).

Spatial variation in water quality can be a result of the interaction of both natural and human-induced catchment characteristics (Varanka et al., 2015). Natural and anthropogenic landscape characteristics often have high cross-correlations. Catchment climate and topography are correlated with land use (Barrientos & Iroumé, 2018; Zhao et al., 2015). Catchments with flat and gentle slopes typically tend to have a higher proportion of cropping agriculture (Melland et al., 2012; Okoba & Sterk, 2010). This might result in more sediment and nutrient exported from these catchments (Ye et al., 2009; Yevenes et al., 2016). The potentially high cross-correlation among catchment characteristics makes it difficult to distinguish the relative importance and individual role of each characteristic in influencing the spatial variation in water quality.

2.2.2 Temporal variability in water quality

Within a catchment, water quality can exhibit substantial temporal variability at daily (Brainwood et al., 2004; Meybeck & Moatar, 2012), seasonal (Lewis et al., 2013; Ouyang et al., 2006; Xu et al., 2019a) and inter-annual (Fabricius et al., 2013; Zhuo et al., 2016) timescales. This variability has typically been linked with changes in hydroclimatic conditions (e.g., Table 2-1, discharge, air temperature and rainfall) among other conditions (e.g. changes in vegetation cover/land use) (Guo et al., 2018; Guo et al., 2019b; Hrachowitz et al., 2016; Jordan et al., 1997; Mosley, 2015; Scanlon et al., 2007; Schilling et al., 2017).

2.2.2.1 Catchment hydrology

Catchment hydrological conditions can have a direct role in determining pollutant source, mobilisation and delivery. Among these temporally varying factors, extensive investigation has been undertaken to understand the relationship between temporal changes in water quality concentration and discharge. Instream water quality can rapidly respond to short-term changes in flow (Allan et al., 1997b). The changes and relative contributions in the water source can result in variability in water quality, that is, storm flows can contain both surface and subsurface runoff (Todd & Mays, 1980), or multiple subsurface sources (Hrachowitz et al., 2016).

For natural surface water systems, constituents can be sourced during multiple flow conditions (e.g., high flows, low flows, cease-to-flows), each of which can have a specific influence on water quality through ecological and geomorphological functions (Bunn & Arthington, 2002). For instance, low flows can provide warm and clear conditions that lead to more rapid nutrient cycling and primary production. This can enhance nutrient removal from watercourses through uptake by riparian vegetation via plant assimilation (Johnston, 1991; Stephenson & Shabman, 2017). On the other hand, higher flows can provide the dilution of ions and toxins, and the supply of nutrients and carbon to support the ecological systems (Liu et al., 2016). Cease-to-flow periods in intermittent and ephemeral streams can dry out the sediments, releasing carbon and nutrients that are available to flora and fauna when flows return (Nilsson & Malm-Renöfält, 2008). In addition, the quality of groundwater can vary in time and space, typically with higher salinity, metal and dissolved nutrient levels than surface water (Kaman et al., 2016; Yan et al., 2015). Therefore, water quality in waterways can differ depending on the relative amount of groundwater contributions from different sources to surface streams.

The mobilisation of pollutants is related to the natural flow regimes in a catchment. This involves a number of physical processes (e.g., reaeration, adsorption, dilution, sedimentation and erosion) occurring in natural streams (Ayers & Westcot, 1985; Letterman, 1999; Melching & Flores, 1999). Among these processes, dilution and sedimentation and erosion are of great significance in terms of the pollutant dynamics at the catchment scale. With the exception of sediments and sediment associated pollutants, concentrations are usually lower when there is more water in streams (Floehr et al., 2013; Keller et al., 2014; Métadier & Bertrand-Krajewski, 2012). This dilution effect can lower the concentrations of ions, toxins and other dissolved substances, especially for salinity (Pai et al., 2015). Sedimentation is an in-situ process that takes place when the velocities drop (i.e., low transport capacity), allowing suspended particles to settle out. Water clarity can increase accordingly, which is essential for aquatic plants that require light for photosynthesis. In high-saline environments, such as estuaries, fine particles can be aggregated into large particles that settle by means of flocculation (Anthony, 1999; Fabricius & Wolanski, 2000; Jouon et al., 2008).

In addition, surface runoff is a driving force in the soil erosion process. Erosion can result in top soil loss and land degradation, leading to high levels of turbidity in receiving waters (Ongley, 1996). In terms of stream sediment concentrations, transport and delivery are also critical. Suspended solids can be either transported or deposited through the river network under different flow conditions (Prosser et al., 2001). The significance of sediment transport is not only due to its impact on the health of ecosystems (e.g., affecting primary productivity through light penetration and nutrient availability) (Carr et al., 2010; Schallenberg & Burns, 2004), but interactions among stream channels, floodplains and the estuarine marine ecosystems (Prosser et al., 2001). In addition to the impact on sediment and turbidity, erosion can be important for other constituents, including nutrient species in particulate forms. Typically, most of the phosphorus in a stream is adsorbed on the surface of the mineral grains (Byers et al., 2005). Noting that particulate N is also often significant, the supply of nitrogen and particularly phosphorus downstream is often closely related to the transport and transformation of the organic and inorganic sediments (Drever, 1988).

Hydrological transport via surface and subsurface runoff is a key mechanism that determines pollutant delivery and transport in catchments (Hrachowitz et al., 2016; Rode et al., 2010; Vidon et al., 2010). The hydrological transport process can also have a direct impact on the fate of solutes, along with biogeochemical processes (Basu et al., 2011; Thompson et al., 2011). Statistical analyses have been used to investigate long-term concentration and discharge monitoring data, to provide an understanding of processes controlling pollutant delivery at the catchment scale (Basu et al., 2010; Basu et al., 2011; Jawitz & Mitchell, 2011).

Power law functions have commonly been used to describe the relation between concentration and discharge (Cvetkovic et al., 1998; Jawitz et al., 2003):

$$\ln C = \ln a + \beta \ln Q + \varepsilon \qquad \text{Equation 2-1}$$

where C is the concentration, Q is the discharge, ε is random error, a and β are fitted coefficients. C and Q are assumed to follow a lognormal distribution. The exploration of fitted parameters is useful for understanding the constituent export behaviour (Zhang, 2018). A constituent with a β close to 0 can be defined as chemostatic behaviour (i.e., concentrations are stable over a large range of flows, $|\beta| < 0.1$) and β away from 0 defined as chemodynamic (i.e., concentration change is larger than the flow change, $|\beta| > 0.1$ with either dilution or concentration) (Godsey et al., 2009). However, this method might lead to incorrect interpretation because when β is close to zero (i.e., there is no or a minimal degree of correlation between discharge and concentration), there is no supporting evidence for explaining the dynamics of constituents (Thompson et al., 2011). Thus, the comparison of variability in both discharge and concentration would be more useful. A metric defined as the ratio of the coefficient of variations (CV) of concentration and discharge has been commonly used to infer the solute behaviour within catchments (Duncan et al., 2017; Musolff et al., 2015; Thompson et al., 2011),

$$\frac{CV_C}{CV_Q} = \frac{\mu_Q}{\mu_C}\frac{\sigma_C}{\sigma_Q} \qquad \text{Equation 2-2}$$

where μ and σ are the mean and standard deviation, respectively. When variability in discharge is lower than that of concentration (chemodynamic conditions), pollutants tend to be more reactive, but when there is temporal variability in discharge (chemostatic conditions), pollutants are easily mobilised or diluted. Jointly assessing slope term β (Equation 2-1) and the ratio of the coefficient of variations of concentration and discharge (Equation 2-2) gives more insight into the export characteristics (Figure 2-1). For example, by using this approach, a chemodynamic behaviour was found for TSS and NH_4, while major ions showed strong chemostatic (dilution), in nine neighbouring catchments in Central Germany (Musolff et al., 2015). Legacy store also controls the constituent processes, including mobilisation and transport, along with high reactivity (orange region in Figure 2-1[b]), especially for dissolved nutrients (Basu et al., 2011; Minaudo et al., 2019).

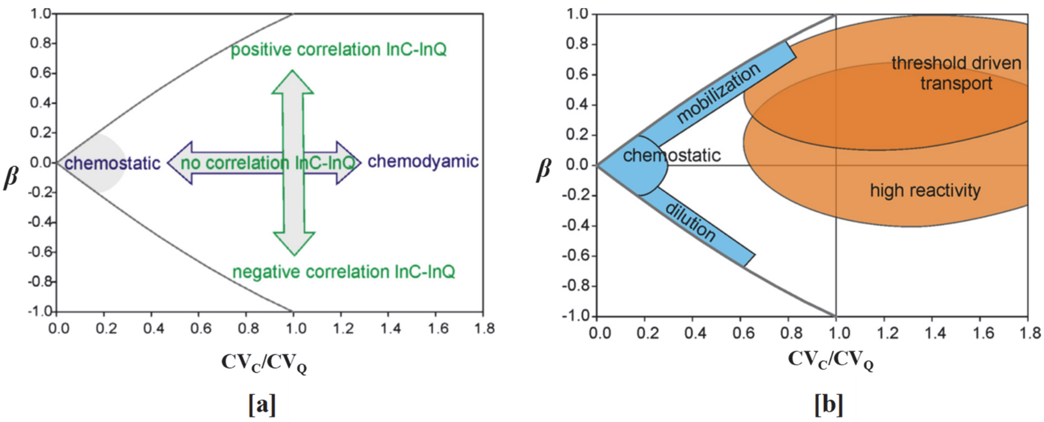

Figure 2-1. Processes leading to characteristic patterns in pollutant export behaviour; (a) general classification of β and CV_C/CV_Q; (b) more detailed processes: blue areas - processes described by the relationship between pollutant sources and discharge; orange areas – strong chemodynamics export regime controlled by additional processes. Adapted from Musolff et al. (2015).

Other hydrological conditions, such as soil water content, can also affect the pollutant dynamics in a catchment (Blaen et al., 2017; Cooper & Hiscock, 2019;

Hrachowitz et al., 2015). The temporal variation in hydrological connectivity (controlled by soil water content) between sources of solutes and flow pathways drives pollutant delivery (Hrachowitz et al., 2016). This variation can also determine the contact time between fixed and mobile phases of solutes, which has an important impact on biogeochemical reactions (Maher & Chamberlain, 2014). Studies have illustrated that a high degree of hydrological connectivity before the event can create a link between water quality variability and the heterogeneity in the source and pathways of pollutants (Jarvie et al., 2008; Jordan et al., 1997; Sebestyen et al., 2008).

2.2.2.2 Catchment weather conditions

Weather variations (e.g., seasonal changes in rainfall and temperature) can be an important factor for driving temporally varying pollutant sources and mobilisation processes. Changes in weather conditions can have greater impacts on sediments and nutrients (i.e., non-conservative substances) through hydrological transport (Section 2.2.2.1) and biogeochemical processes (Meybeck et al., 1996).

Catchment weather conditions can partly determine the source of pollutants within a catchment (Fan & Shibata, 2015; Molina-Navarro et al., 2018; Mosley, 2015). For instance, higher temperatures have been typically linked to lower nutrient stores in catchments (Lintern et al., 2018a). This is attributed to nutrient uptake by vegetation growth, which is enhanced at optimal temperatures (Neitsch et al., 2005; Picard et al., 2005). A higher temperature can also favour the activity of bacterial denitrification, thus enhancing the denitrification rate and attenuating nitrogen (Burt et al., 1999; Duff & Triska, 1990; Pinay et al., 2009; Weller et al., 1994). In addition, in areas with higher rainfall, the wetter conditions can facilitate the reduction of NO_3^- to N_2 through denitrification, under anaerobic environments (i.e., when O_2 is limited) (Creed & Beall, 2009; Zhou et al., 2014). For instance, oxidised nitrogen (NO_X) concentration in 44 water quality monitoring sites in Japan was found to be positively proportional to the presence of the amount of wetland and rainfall (Hayakawa et al., 2006).

Catchment weather conditions can also affect pollutant mobilisation. An increase in temperature likely enhances the weathering processes of the bedrocks (Bouchard & Jolicoeur, 2000). This usually leads to increased sediment and nutrient concentrations in receiving waters (Hattanji & Onda, 2004; Pelletier & Baker, 2011). Higher temperatures have also been linked to the mineralization and decomposition of nutrients, which can increase the amount of mobilised pollutants in both soils and streams (Dagg et al., 2004; Liao et al., 2008; Mosier et al., 2004; Sims & Sharpley, 2005). In addition, the intensity and amount of rainfall are critical to soil erosion rates (Römkens et al., 2002). Sediments and nutrients (in particulate forms) are prone to be mobilised through rainfall, with higher erosivity on a ground surface with lower roughness (e.g., low vegetation cover) (Battany & Grismer, 2000; Pielke Sr et al., 2007). For instance, fine sediment generation was positively correlated with rainfall intensity and erosivity in a catchment in New Zealand (Fahey & Coker, 1992).

2.2.2.3 Catchment ground cover

Seasonal changes in catchment ground cover (types and amount of vegetation) can have a direct impact on source and mobilisation of sediments and nutrients (Kamarinas et al., 2016; Rhoades et al., 2019; Shi et al., 2017; Wang et al., 2016). Many studies have found that such changes in ground cover are linked to temporal changes in riverine water quantity and quality (Bosch & Hewlett, 1982; Boven et al., 2008; Turner & Rabalais, 2003; Zhang et al., 2001). Denser vegetation can reduce the erosive effect of rainfall on soil, thus reducing soil erosion from hillslopes, gullies and streambanks (Thorburn & Wilkinson, 2013). In addition, the ground vegetation condition can affect the amount of nutrients available in catchments (Harris, 2001; Lintern et al., 2018a). Other positive effects of vegetation cover for maintaining water quality relate to sediment trapping (Braskerud, 2001; Gonzales et al., 2018) and transformation of dissolved nutrients by biogeochemical processes (Conley, 1999; McMillan & Noe, 2017).

At the terrestrial – aquatic interface, riparian vegetation growing along stream banks can have significant effects on the transport of eroded sediment and associated nutrients into streams (Fu & Burgher, 2015; Hill, 1996; Karssies & Prosser, 1999; Li et al., 2013; Lowrance et al., 1997). Specifically, riparian buffer zones can effectively stabilise stream banks and trap eroded sediment by reducing the velocity of runoff and encouraging the deposition of particle-bound nutrients and pesticides (Bu et al., 2016; Schmitt et al., 1999). TP retention includes processes as such sedimentation of particulate phosphorus, and plant uptake of dissolved phosphorus (Doyle et al., 2003; Lowrance et al., 1997). Also, riparian vegetation can provide anoxic saturated environments, allowing dissolved N removal by processes such as nitrification/denitrification (Parkyn, 2004). The beneficial effect of a riparian buffer depends on not only the types and loads of pollutants, but also on the characteristics of the riparian zone, such as buffer width and slope, vegetation species, as well as the buffer installation and management methods (Muñoz-Carpena et al., 2010). A number of simulation and field experiments have demonstrated that, at runoff event scale, the considerable reduction in sediment (up to 98%) and nutrients (up to 92%) from agriculture that has resulted from the effect of riparian buffer (Mankin et al., 2007; Syversen, 2005).

2.3 Riverine Water Quality Issues

2.3.1 Non-point source pollution

Globally, terrestrial non-point source pollutant (NPS) is one of the main threats to riverine water quality (Giri et al., 2016; Ouyang et al., 2018). NPS is typically associated with a wide range of human activities and does not have one obvious entry point into receiving waterbodies (Ongley, 1996). It includes terrestrial runoff from agricultural and urban land uses, atmospheric deposition, and effects of road or railway transportation (Cabe & Herriges, 1992; Ongley et al., 2010). Agriculture is one of the most significant contributors of NPS due to the large areas involved together with accelerated soil erosion and intensive application of fertiliser and pesticides (McCoy et al., 2015; Palis et al., 1990). In North America, NPS has been identified as a key driver of water quality degradation and has been investigated intensively since the 1970s, following the eutrophication crisis of the Great Lakes in the 1960s (Mills et al., 1993; Patalas, 1972). Likewise, with the rapid economic and social development in China from the 1980's to 2006, it is estimated that agricultural NPS accounts for 50% and 80% of the total nitrogen and phosphorus pollutant load, respectively, in the Yellow River Basin (Han et al., 2006). Among different types of NPS, suspended solids, nutrients and pesticides are of great concern due to their high ecological and environmental impacts on marine ecosystems (Bainbridge et al., 2009b; Devlin & Brodie, 2005).

Suspended sediments, especially following extreme flood events, can increase turbidity in inshore waters and reduce the light available for corals and seagrass meadows (Hairsine, 2017). At the same time, increases in fine particulate sediments and organic rich flocculent masses can smother marine organisms (Brodie et al., 2013b). The identification of sediment sources draining into streams and marine ecosystems is essential for sediment management (Bainbridge et al., 2018; Bartley et al., 2014a; Hughes et al., 2011). There are three key soil erosion mechanisms, namely hillslope, gully and streambank erosion (Fox et al., 2016; Fox & Wilson, 2010; Renard et al., 1991; Valentin et al., 2005). The interaction between soil property, precipitation (i.e., duration and intensity) and land use and land management practices determine erosion processes, which in turn affects sediment concentrations in streams (Arnold et al., 1995; Nu-Fang et al., 2011; Suif et al., 2016).

Nutrients (e.g., nitrogen [N] and phosphorus [P]) are essential for the agricultural industry and excessive nutrient inputs have adverse effects on aquatic ecosystems (Brodie et al., 2017a; Brodie et al., 2017b; Garzon-Garcia et al., 2018; Helton et al., 2011; Kroon et al., 2016). Excessive enrichment from agricultural runoff in waterbodies may lead to eutrophication (e.g., associated with algal bloom and fish kills) (Boesch et al., 2001; Dodds & Smith, 2016). Biological or agricultural nutrient fixation, atmospheric deposition, livestock manure and fertiliser application are major nutrient inputs into catchments (Swaney et al., 2012). Among these inputs, nitrogenous fertiliser is the most important input in most agricultural land (Balls et al., 1995; Connolly et al., 2015; Lu & Tian, 2017).

Pesticides include herbicides, insecticides and other pest and weed control chemicals (Olafson, 1978; Smalling et al., 2015; Thorburn et al., 2013). Pesticides have severe toxicity for aquatic bio-systems (El-Nahhal, 2018; Oliveira et al., 2015). These persistent toxic compounds are typically associated with long half-life, high mobility, resulting in high risk for both surface and groundwater (Carvalho et al., 2002; Derakhshan et al., 2018). Volatilisation and subsequent chemical and biological decay are principal processes for removal of pesticides both in soil and water bodies (Rüdel, 1997; van der Werf, 1996).

In addition to the abovementioned three main types of NPS, salinity has been a public concern in recent decades (Ayache et al., 2019; Foster et al., 2018; Smith et al., 2010). Regional groundwater is the largest contributor to high salinity, particular in the lowlands of dry catchments (Cartwright et al., 2017; Gil-Márquez et al., 2017; Jolly et al., 2001; Kang & Jackson, 2016). Salinization of soils is a severe land degradation issue, leading to a negative impact on crop productivity in parts of Australia and elsewhere in the world (Bell et al., 1993; Pérez-Alfocea et al., 2010; Vinogradova et al., 2019; Yeo, 1998).

2.3.2 Water quality status in the GBR catchments

The Great Barrier Reef (GBR) lagoon has received elevated levels of pollutants from the adjacent catchments since European settlement, which began in the 1850s (Brodie et al., 2012; Hunter & Walton, 2008; Kroon et al., 2016; McKergow et al., 2005b). As in other parts of the world, diffuse sources from agricultural activities have been the one of the main contributors to waterway pollution in the GBR catchments (Brodie et al., 2013b).

In this section, the detrimental effects of excessive pollutant load in the GBR marine ecosystems and previous studies on the generation and load estimation of major pollutants (e.g., sediment, nutrients and pesticides) in the GBR catchments are presented. Figure 2-2 demonstrates a conceptual pathway of the movement of pollutants from catchments, indicating the movement and partitioning of pollutants between the water column, marine sediments, and marine biota.

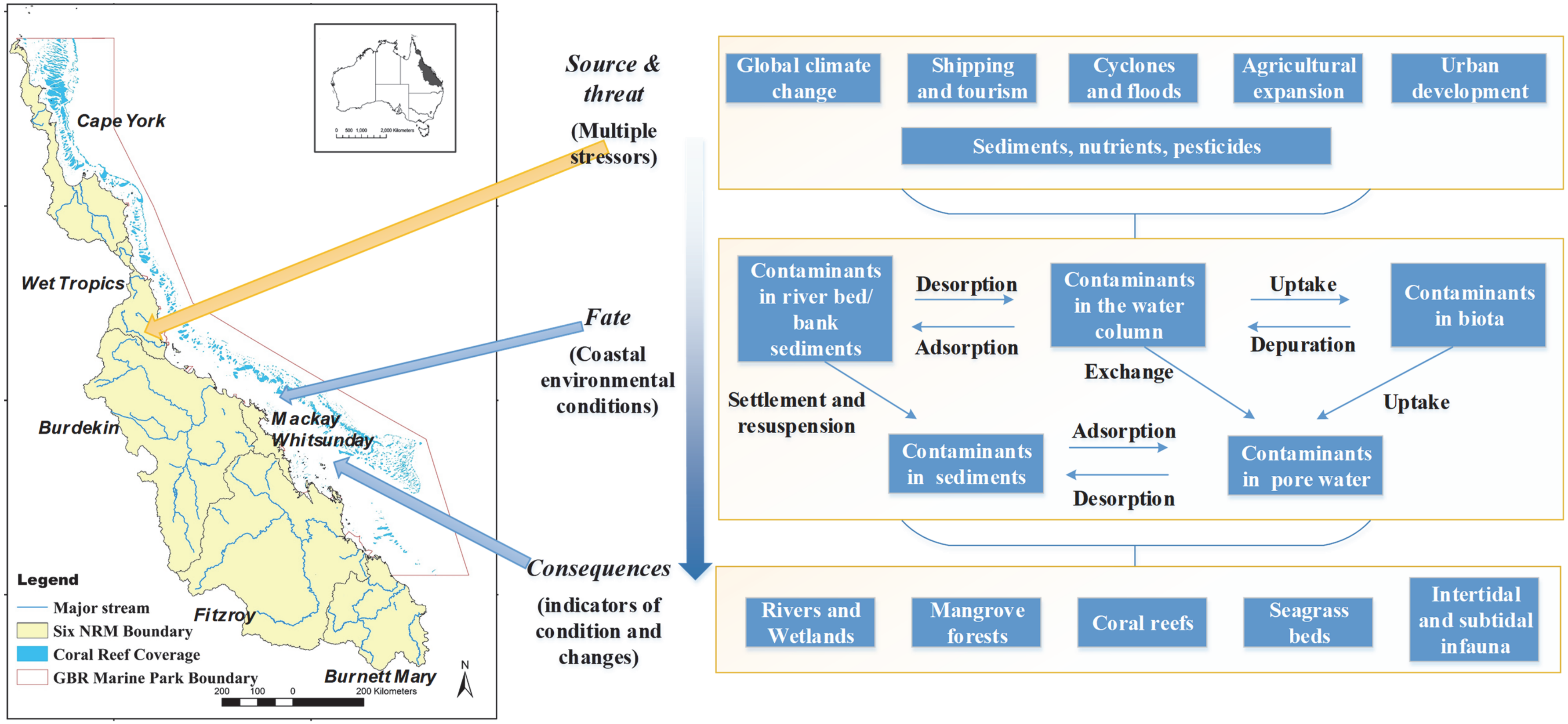

Figure 2-2. The GBR lagoon process-based conceptual model of pollutant source/threat, fate and consequences. Source, fate and consequences are associated with areas in the GBR lagoon and catchments. Adapted from Haynes et al. (2007)

2.3.2.1 Suspended sediments

Suspended sediments draining from the GBR catchments into the coral reef lagoon are one of the most significant pollutants, leading to poor marine water quality and decline in coral cover (Goatley et al., 2016; Gordon et al., 2016; MacNeil et al., 2019; Wenger et al., 2016).

The generation of suspended fine sediment loads in the GBR catchments is primarily a result of erosion processes, which can vary in space and time due to their sensitivity to climatic and hydrological drivers, including rainfall and runoff (Thorburn et al., 2013). Sediment loads can also be affected by anthropogenic activities, particularly agricultural management practices that influence vegetation and soil cover and that physically disturb the soil such as cultivation and compaction. The Burdekin and Fitzroy regions (described in Section 3.3.1) pose the most significant water quality risk to the GBR ecosystems due to their large annual TSS loads (Brodie et al., 2003; Devlin & Brodie, 2005; Waterhouse et al., 2012). This can be attributed to the low relief and relatively dry climate of the inland GBR catchments (Thorburn et al., 2013). Sediment loads in the Burdekin and Fitzroy regions have been relatively high compared with other GBR catchments and the majority of catchments in a global database (Figure 2-3 [a]). However, sediment yields are relatively low for these two regions (Figure 2-3 [b]). This is due to the low annual rainfall/runoff associated with lower erosion rates (Meinke & Stone, 2005; Petheram et al., 2008).

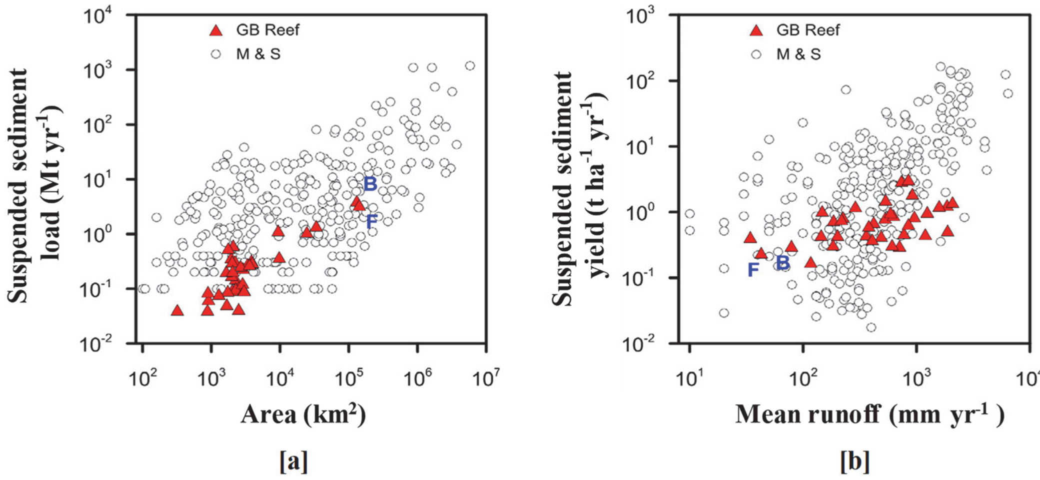

Figure 2-3. Mean annual suspended sediment load (a) and yield (b) for GBR (red triangles) and global (white circles) catchments. Letters in blue (F and B) refer to the largest catchments of Fitzroy (F) and Burdekin (B). M & S refers to the global data from Milliman and Syvitski (1992). Modified from Thorburn et al. (2013).

Modelling has been undertaken to identify the sediment budget in the GBR catchments. McKergow et al. (2005b) used a spatially distributed sediment model and estimated that hillslope erosion was the major erosion contributor to long-term annual sediment exports, accounting for 63% of annual average sediment loads. Gully and streambank erosions contributed around 28% and 9% of sediment loads, respectively. However, this may have been an underestimation of hillslope erosion rates, due to a lack of understanding of gully and streambank erosion processes, as well as limited spatial data for riverbank erosion. Sediment source tracing studies carried out in the Burdekin catchment in 2006/07 indicated that approximately 77% to 89% of fine sediment originated from subsurface soils and that gully erosion was the key process generally leading to the erosion of sub-surface soil (Wilkinson et al., 2013).

A more recent study estimated that gully and streambank erosions were responsible for over 50% of the total erosion in the GBR in 2012/13 (Waters et al., 2014). Gully network density is one of the influential factors that can influence the extent of gully erosion, and in the GBR catchments gully erosion is believed to be a dominant sediment source from subsurface soil given that there is an active and dense gully network (Thorburn & Wilkinson, 2013). In addition, the contribution of streambank erosion becomes greater during high flow period, compared to hillslope and gully erosion processes, especially within coastal catchments and floodplains. All three types of erosion are strongly influenced by surface runoff and land cover at sites where erosion tends to occur (Bartley et al., 2006; Koci et al., 2019; Silburn et al., 2011; Wilkinson et al., 2018; Wilkinson et al., 2015). Therefore, an increase in surface runoff can intensify both hillslope and gully erosion rates (Oostwoud Wijdenes & Bryan, 2001), and can also enhance streambank erosion (Dalzell & Mulla, 2018; Rutherfurd, 2000).

2.3.2.2 Nutrients

There is a clear relationship between N exports from the GBR catchments and N fertiliser application intensity (Thorburn et al., 2013). In addition, N surpluses after fertiliser application were the key driver of dissolved inorganic nitrogen (DIN) losses from agricultural land to streams (Thorburn et al., 2013).

The average N fertiliser application intensity varies across the GBR catchments, depending on crop types (Fraser et al., 2017; Kandulu et al., 2018; Thorburn & Wilkinson, 2013; Thorburn et al., 2013). Typically, the coastal regions have N fertiliser application rates, at > 8 kg ha^{-1} yr^{-1} (Thorburn et al., 2013). This can be explained by the fact that climate in these regions not limit productivity of sugarcane and horticultural cropping, resulting in a relatively high rate of N fertiliser application. It has been estimated that the average N fertiliser application rate for sugarcane in the GBR catchments is around 160 kg ha^{-1} yr^{-1} in the year of 2013 (Bell, 2014). In contrast, there has been < 4 kg ha^{-1} yr^{-1} of N fertiliser applied in the inland regions. In these regions, sugarcane and horticultural cropping constitute less than 2% of the catchment areas (Devlin & Brodie, 2005; Liu et al., 2018).

The majority of DIN exports usually occurs in surface runoff and deep drainage (leaching) to groundwater, and losses of DIN via leaching are highly relevant to N fertiliser application in the GBR catchments (Onderka et al., 2012; Webster et al., 2012; Wooldridge, 2009). Studies indicated that surface runoff associated with timing of fertiliser application was a key factor affecting DIN concentration. (Fraser et al., 2017; Mitchell et al., 2009). In addition, in humid tropical regions in the GBR catchments, deep drainage was the dominant pathway for DIN transport (Armour et al., 2013). The modelling study in the Mackay Whitsunday region indicated that DIN losses through deep drainage (3049 t yr^{-1}) was much higher than via runoff (204 t yr^{-1}) (Biggs et al., 2013). Two processes are most likely responsible for high N exports through leaching in these land uses. First, at sites dominated by sugarcane and banana, there is a high mineralisation rate of organic matter in soil, leading to the loss of substantial N through deep drainage (Armour et al., 2013). Second, over-application of N fertiliser provides excessive DIN that crops cannot uptake, generating high N surpluses (Thorburn & Wilkinson, 2013).

Concentrations of particulate forms of nutrients (i.e., particulate nitrogen (PN) and particulate phosphorus (PP)) increase when floods result in a significant proportion of particulate nutrients and sediments being re-suspended and transported to receiving waters (Lloyd et al., 2016; Schaffelke et al., 2012; Sherriff et al., 2015). However, PN and PP may not be significantly correlated with discharge due to sediment-bounded phosphorous has similar processes with suspended solid loads, which are changing dramatically during flood events (Devlin & Brodie, 2005; Ziegler et al., 2016). Under most circumstances, PN and PP are the highest in the dry catchments (Burdekin and Fitzroy regions), and relatively low in clearer rivers in the Wet Tropics (Furnas, 2003; Waters et al., 2014).

2.3.2.3 Salinity

Stream salinity has been a public concern in Australia since the early 1980s when it was first noticed that salinity levels exceeded drinkable standards in the lower Murray (Blackmore & Connell, 1997). Unlike many other Australian catchments (e.g., in Western Australia, Victoria and New South Wales), high salinity typically has not been a widespread issue in the GBR catchments (Bell et al., 1993; Blinn & Bailey, 2001; van Dijk et al., 2007). However, long-term biological oceanographic studies have found an association between low salinity and elevated nutrients and pesticide concentration in flood plumes in the GBR lagoon (Devlin & Brodie, 2005; Shaw et al., 2012). When runoff increases, this leads to intensive low salinity events in the lagoon, which is a major cause of coral mortality, especially on coastal reefs close to major river systems (Chui & Ang, 2015; Dias et al., 2019; Röthig et al., 2016; Van Woesik et al., 1995).

2.3.2.4 Pesticides

Currently, photosystem II (PSII) inhibiting herbicides are widely applied in the GBR catchments and they have been detected in water flowing into the GBR lagoon at increasing levels (De Valck & Rolfe, 2018; Haynes et al., 2000; Lewis et al., 2009; Mercurio et al., 2018; Smith et al., 2012). Sugarcane has been the largest herbicide contributor in the GBR catchment, generating approximately 94% of the total herbicide load in 2012/2013 (Waters et al., 2014). Typical herbicides used in the GBR catchments are soil residual herbicides, such as ametryn, atrazine, diuron, hexazinone, and tebuthiuron, with the half-lives ranging from 30 to 1,000 days (Lewis et al., 2014).

It is worth noting that even though pesticides have been identified as important water quality parameters in the context of the GBR catchments, they are excluded from the analyses of this study. This is because the types of pesticide applied have evolved over recent years. For example, there have been further restrictions in the use of diuron since 2012, following regulatory changes (APVMA, 2014). This has resulted in alternate pesticides being used in different years and regions, which makes it challenging to gain a consistent understanding of individual pesticides (Lewis et al., 2014). In addition, the monitoring records for pesticides often contain substantial proportions below the limits of detection (LOD) measurements, resulting in large uncertainty in the observations (Barr et al., 2006). The exclusion of pesticides in this thesis does not mean pesticides are not a problem and that we need to develop ways of understanding their fate, transport and effects better.

2.3.3 Summary

Riverine water quality issues in the GBR catchment lead to degradation of coral reef in the GBR lagoon. Agricultural NPS has been identified as a major contributor of pollutant loads. Through water quality monitoring and modelling, a great amount of effort has been made to quantify the loads of pollutants discharging into the GBR lagoon (Brodie et al., 2013c; Waterhouse et al., 2017; Waters et al., 2014). However, the water quality of surface runoff draining into the GBR lagoon has not improved substantially, and deterioration is likely to continue in the future (Brodie et al., 2013c; Waterhouse et al., 2017; Waters et al., 2014). Therefore, to make effective water quality management strategies, we need to understand the controlling factors affecting water quality dynamics among different constituents.

The existing literature indicates that there is a wide range of potential factors that can affect catchment water quality dynamics. In terms of the investigation of spatial variation in water quality, studies carried out in the GBR catchments to date have either focused on a limited number of catchment landscape characteristics (e.g., land uses, see Hunter and Walton (2008) and Kroon et al. (2016)), or have been limited to small scales (e.g., paddock or sub-catchment scale studies, see Armour et al. (2013), Bainbridge et al. (2009a) and Bainbridge et al. (2009b)). There is a lack of in-depth understanding of the relative importance of natural and anthropogenic catchment characteristics effects on spatial differences in water quality. In addition, even though previous studies have attempted to improve our understanding of water quality temporal dynamics (Bartley et al., 2014a; Gladish et al., 2016; Kroon et al., 2012), the effects of temporal variation in hydroclimatic conditions and vegetation cover on the temporal changes in water quality in the GBR is limited to a number of sites or a restrained investigation region. The temporal controls on water quality dynamics across large-scale GBR catchments or other regions of the world still require further investigation. To close this gap, both water quality monitoring data and modelling approaches are needed to improve our understanding of water quality dynamics.

2.4 Catchment Water Quality Modelling

The modelling of non-point source pollutants has gained increasing attention regionally and globally (Heng & Nikolaidis, 1998; Miller et al., 2014). Based on the complexity of the key processes considered and the temporal and spatial scales of these processes, catchment water quality models can be divided into three main types: statistical models, deterministic (process/physically-based) models, and hybrid models (Fu et al., 2019; Gladish et al., 2016; Letcher et al., 2002; Mitchell & McDonald, 1995; Wellen et al., 2015). Figure 2-4 summarizes several commonly used catchment water quality models. The statistical models simplify the hydrological or biogeochemical processes using relatively simple functional forms and assume limited a priori understanding of processes. In contrast, deterministic (or process-based) models use more complex mass-balance structures, describing the water quality source, mobilisation and transport processes. Typically, these catchment water quality models (e.g., statistical, deterministic and hybrid) aim to predict pollutant concentrations or loads delivered to streams on different time steps, ranging from sub-daily to annually (Bonhomme & Petrucci, 2017; Cox, 2003; Faruk, 2010; Kuhnert et al., 2012; Tsakiris & Alexakis, 2012).

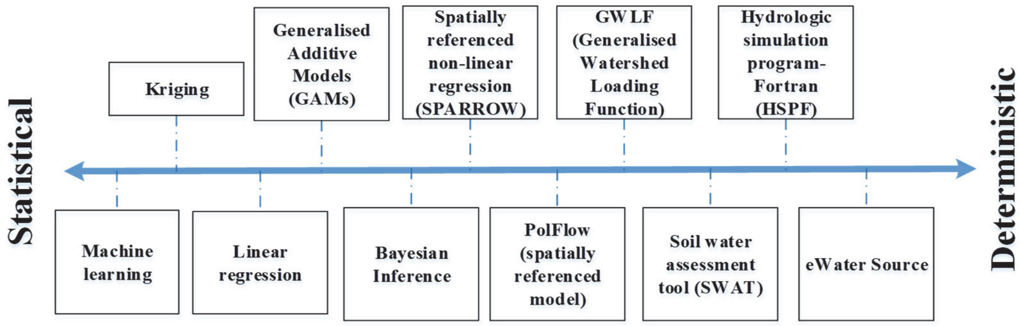

Figure 2-4. Catchment water quality modelling types based on the level of statistical and deterministic (mechanistic) descriptions of pollutant source and biogeochemical processes. Modified from Schwarz et al. (2006).

2.4.1 Statistical water quality modelling

The key concept underlying statistical/empirical model is fitting a linear or nonlinear function to relate water quality responses and catchment sources and landscape properties. The benefits of statistical models include: a) a relatively simple mathematical structure; b) ability to quantify predictive uncertainty (Kasiviswanathan & Sudheer, 2013; Srivastav et al., 2007); and c) the lower requirement for a priori information on distinct processes (Afed Ullah et al., 2018; Letcher et al., 2002; Mainali et al., 2019; Schwarz et al., 2006). Within statistical water quality models, the fully data-driven statistical/machine learning approaches (e.g. neutral networks) have shown a good fit between observation and simulation, but provide limited insights into the understanding of the processes that can influence the transport of pollutants (Hu et al., 2005; Singh et al., 2009). To provide more direct interpretability of physical understanding from statistical/machine learning approaches, Random forests (RF) regression has been used to explore linear and non-linear relationship between water quality (e.g., sediment) and environmental variables (e.g., discharge) in recent years (Chen et al., 2020; Liu et al., 2014; Rodriguez-Galiano et al., 2014). However, sufficient training data and long training period (i.e., high computational costs) are needed to create a trained model with satisfactory predictive ability (Liaw & Wiener, 2002).

Linear regression has been the most frequently used approach to investigate the relationship between landscape characteristics and water quality spatial variation (Afed Ullah et al., 2018; Letcher et al., 2002; Mainali et al., 2019; Schwarz et al., 2006), between concentration and discharge (Bowes et al., 2015; Godsey et al., 2009; Moatar et al., 2017; Musolff et al., 2015), and for water quality response to changes in land use and land cover change (Griffith et al., 2002; Li et al., 2008; Li et al., 2009; Pratt & Chang, 2012; Singh et al., 2013). These investigations have often been based on identifying a 'best model' using forward or backward stepwise variable selection (Hu et al., 2019; Juahir et al., 2011; Ren et al., 2003; Rothwell et al., 2010; Sangani et al., 2015; Singh et al., 2004). One important issue is that predictions derived from the single 'best' statistical model are prone to the problem of model-selection uncertainty, leading to overconfident predictions and misleading inferences of other processes that are not captured (Neuman, 2003; Wintle et al., 2003). A challenge remains regarding model selection, as multiple controlling factors and collinearity in these factors often result in a set of plausible models that have similar predictive power (Whittingham et al., 2006).

The use of weighted regressions on time, discharge, and season (WRTDS) has been widely used in the United States of America (USA) (Hirsch et al., 2010; Moyer et al., 2012; Zhang & Blomquist, 2018; Zhang et al., 2016a). It has been applied to a range of modelling purposes, including the investigation of the spatial and temporal pattern of the sediment and nutrient export at the catchment scale in the Chesapeake Bay in the states of Maryland and Virginia (Zhang & Blomquist, 2018), the examination of the trend in chloride concentration in streams of the conterminous USA (Stets et al., 2018), and the exploration of spatial differences in nitrogen fluxes in response to agricultural land uses and climate change in Iowa, USA (Green et al., 2014). The general modelling framework is,

$$\ln(C) = \beta_0 + \beta_1 t + \beta_2 \ln(Q) + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t) + \varepsilon \quad \text{Equation 2-3}$$

where C is instantaneous concentration, t is time in decimal years, Q is daily discharge, β_i (where i = 1, 2, 3 and 4) are the estimated model coefficients, and ε is an error term. The sin and cos terms represent seasonality. This method is useful for exploring the relationship between concentration, discharge and time at one particular site (i.e., model parameters are calibrated site by site); however, it provides no information on the factors that may drive the spatial variation in water quality among different sites/catchments.

An extended form of Equation 2-3 has been developed by Kuhnert et al. (2012), with an aim to estimate annual sediment load in the Burdekin catchment in the GBR. The concept of this modelling framework involved fitting a flexible generalized additive modelling (GAM) framework for characterising flow and concentration relationships for estimating loads at a water quality monitoring site. An appealing advantage of this approach is its ability to quantify the uncertainties arising from:1) sampling errors in both concentration and discharge; 2) lack of understanding of the underlying hydrological processes; and 3) sampling frequency and sampling time over hydrograph (by introducing a categorical variable in modelling structure to reflect concentration differences between the rising, falling and baseflow of hydrograph over an event).

During the last two decades, more advanced spatial regression models have been used to analyse the complex relationship between land use/cover and water quality. Geographically weighted regression (GWR) models can explain local variation by incorporating spatial coordinates into the regression model, allowing better modelling performance with a higher coefficient of determination (R^2) compared to ordinary least square (OLS) regression (Tu & Xia, 2008). Recently, spatial regression models have been incorporated with Kriging techniques to investigate the impacts of catchment-scale conditions on water quality by modelling the spatial autocorrelation among observations (Chang, 2008; Goovaerts et al., 2005; Hong & Jeon, 2017; Mainali & Chang, 2018; Mainali et al., 2019; McLean et al., 2019). Flow and stream distance can be also integrated by using spatial moving averages to obtain valid covariance matrices for residual autocorrelation models (Ver Hoef et al., 2006). With a sufficient number of observations, spatial regression models can also provide accurate predictions with uncertainty estimations (Wan et al., 2014a; Yang & Jin, 2010). However, only limited information can be gained on the identification of controlling factors affecting the spatial difference in water quality.

The key strengths of statistical water quality models are simplicity and flexibility, while they are often limited by spatially complicated and temporally dynamic ecological processes (Lobell & Burke, 2010; Ouedraogo et al., 2019; Shen et al., 2019). The generalized linear mixed model (GLMM) may provide a flexible stochastic modelling framework that is able to describe complicated processes within a statistical framework (Hwang et al., 2016; McCulloch & Neuhaus, 2005; Qian et al., 2010). However, challenges have remained about realistically accounting for the joint spatiotemporal dependence structure (i.e., typical water quality dynamics) in the random effects term (Wikle, 2003b). Another disadvantage of this approach when dealing with non-linear, inter-correlated water quality parameters, is that the distribution of data tends to be non-Gaussian (Schleiter et al., 1999).

A broader issue with most statistical models is the assumption that the spatial distribution of sources and sinks is homogeneous, which does not distinguish terrestrial from in-stream loss processes and not allow for improvement in the understanding of spatial trends in these processes (Alexander et al., 2002b). This is one reason why statistical models are limited in transferability (i.e., cannot be applied to other catchments or other time periods) and they thus have a low ability to predict under novel conditions which is often required for scenario testing (Wellen et al., 2014b).

Finally, one important issue is that predictions derived from the single 'best' statistical model are prone to the problem of model-selection uncertainty, leading to overconfident predictions and misleading inferences regarding other processes that are not captured (Neuman, 2003; Wintle et al., 2003). A challenge has remained in the method of model selection, as multiple controlling factors and collinearity in these factors have resulted in a set of plausible models that have similar predictive power (Whittingham et al., 2006). To date, there has been limited research jointly addressing model selection uncertainty when predicting water quality spatio-temporal dynamics across different locations (Gladish et al., 2016; Guo et al., 2019a).

2.4.2 Deterministic water quality modelling

Deterministic (process-based) water quality models are based on hydrological and biogeochemical processes that can affect the generation and transport of pollutants into receiving waters. Basically, the hydrological processes are simulated either by equations of mass and momentum conservation for the flow and conservation of mass sediment or by empirical equations (Abbott et al., 1986; Merritt et al., 2003). Deterministic models typically describe the generation of streamflow, and the transport of sediment and soil nutrient cycling separately (Wellen et al., 2015). The components of the models can provide a high temporal resolution of the description of pollutant concentrations in response to climatic variation. The impacts of coarser temporal variability in land use and land management practices have often been superimposed on the more detailed climatic variations (Schwarz et al., 2006). Two widely used deterministic water quality models in large catchments are SWAT (Soil and Water Assessment Tool) (Arnold et al., 1990; Neitsch et al., 2002) and eWater Source Catchments (Carr & Podger, 2012). Both have been applied to solve various water quality management issues.

SWAT is a widely used, physically-based, conceptual and continuous time water quality modelling tool that assesses the impact of land use management and climate on sediment, water and pollutant constituents from non-point agricultural sources in large catchments (Arnold & Fohrer, 2005; Francesconi et al., 2016). SWAT divides a catchment into a number of sub-basins using a digital elevation model (DEM). Sub-basins are represented with one or more hydrologic response units (HRUs). Each HRU has a series of sub-models that can include hydrology, weather, sedimentation, soil temperature, crop growth, nutrients, pesticides and agricultural management. The hydrological and biogeochemical processes are described by mathematical or empirical equations. Therefore, the parameters for these sub-models often have physical meanings, although they may not be measurable. The resulting loads are then routed through the channel network to the basin outlet using a daily time step (Yang et al., 2007).

Source Catchments is a lumped, semi-distributed, conceptual catchment modelling framework that has been widely used in Australia, integrating eco-hydrological modelling tools to support Integrated Water Resources Management (IWRM) (Carr & Podger, 2012). It consists of rainfall-runoff models and pollutant export and routing models to simulate catchment water quantity and water quality, typically operating at a daily timestep. A node link network is created to represent the sub-basins and the stream network. Different land uses are defined by functional units (equivalent to HRUs) (Carroll et al., 2012). Sediment and nutrient generation and filtering are constructed using models such as SedNet/ANNEX (Wilkinson et al., 2014). Source Catchments provides a flexible and extendable platform to incorporate with other modelling tools to predict the processes of flow and instream constituents from headwaters to the sea. For example, RUSLE and SedNet/ANNEX have been used to simulate soil and streambank erosion for assessing the impact of agricultural management practices in the GBR catchments (Waters et al., 2014). It has also been applied in the Australian Murray-Darling River Basin to optimise water management and delivery for agriculture, industry and environmental uses (Ly et al., 2019).

The complexity of deterministic models such as SWAT and Source Catchments results in intensive data and calibration requirements, and large-scale application has been limited (Abbaspour et al., 2015; Arnold & Fohrer, 2005). If observations are insufficient, reaction rates and other process components cannot be calibrated directly. Instead, they have to be estimated based on assumptions (Schwarz et al., 2006), compromising model accuracy. Moreover, it is often difficult to quantify model uncertainties and to identify unique models with sensitive and/or uncorrelated parameters. These models may have large uncertainties in the interpretability of the parameters and their characterization of the effects of specific processes (Wade et al., 2002), such as denitrification in streams (Filoso et al., 2004). However, these uncertainties are not assessed.

Complex physically based models can provide water resource managers with valuable insights into water quality behaviours under varying scenarios. However, there has been a growing concern about the sufficiency of observed datasets and understanding of biogeochemical processes necessary to support model applications (Beven, 2002; Chen et al., 2017; Hrachowitz et al., 2016; Jakeman & Hornberger, 1993; Li et al., 2018b; Qi et al., 2019). An increase in the number of model parameters beyond a certain limit has tended to result in only marginal increases in predictive accuracy and interpretability (Hill, 1998). Also, once complexity increases, the models require intensive calibration and validation, while model parameters may be increasingly sensitive to geographical locations (El-Kaddah & Carey, 2004; Filoso et al., 2004). This leads to difficulties in applying deterministic models over a large region consisting multiple catchments (Abbaspour et al., 2015). Furthermore, typically, calibration for the hydrological component of process-based models has only been performed at the basin outlet, leading to an overconfident evaluation of model capability to simulate internal dynamics for the entire basin, including the source and transport of pollutants and land use impacts (Wellen et al., 2015). This issue of lumping of local hydrological processes with basin scale lumped parameters reduces the models' ability to predict new data, even when the model may fit the observations relatively well (Pelletier, 2012; Sun et al., 2017; Tsuruta et al., 2018).

2.4.3 Hybrid water quality modelling

Due to the complexity of the water quality processes and limited data availability, there has been an emerging trend to combine physically-based models with statistical frameworks (Wellen et al., 2014a). The spatially referenced regressions on watershed attributes (SPARROW) modelling approach has been one of the most frequently applied hybrid water quality models (Schwarz et al., 2006). The deterministic mass transport component includes surface water flow paths, non-conservative transport processes, and mass-balance constraints on model inputs (sources), losses (terrestrial and aquatic losses/sinks) and outputs (nutrient flux). Statistical methods are used to explain instream measurements of water quality in relation to upstream sources and catchment characteristics (e.g., soil type and land cover) (Preston et al., 2009).

SPARROW expresses average nutrient loads as nonlinear functions of catchment characteristics, including point and nonpoint nutrient sources and delivery efficiencies (Alexander et al., 2002a; Alexander et al., 2001). The annual stream pollutant load is estimated for a series of catchments that contain defined water bodies, including stream reaches and reservoirs defined by a drainage network. Flow monitoring data, nutrient monitoring data and characteristics of the catchment are spatially referenced for the nutrient load estimation. SPARROW has been successfully applied in the USA and New Zealand (Preston et al., 2009; Schwarz et al., 2006) at national and regional levels to provide annual nutrient yields. The results have been important for water resource managers in implementing effective management plans (Elliott et al., 2005; Moore et al., 2004; Preston & Brakebill, 1999). For example, SPARROW has provided estimates of the delivery of loads from 62,000 stream reaches that contribute to major rivers and estuaries in the USA. Findings from a regional SPARROW study by Alexander et al. (2007) implied that agriculture was the principal nutrient contributor to the Gulf of Mexico. These modelling outcomes have improved the understanding of the sources and transport of nutrients to the downstream receiving waters (Smith et al., 1997).

One limitation of SPARROW is that it focuses on predicting spatial differences in water quality, rather than the temporal variability of the constituent dynamics. Model estimates from SPARROW for small catchments are likely to have a high level of uncertainty (Robertson et al., 2009). Another limitation is that, in a nonlinear regression configuration, identical sets of model coefficients (e.g., the nutrient delivery rates) have been used for different sub-catchments, and that the spatial autocorrelation in observations has not been incorporated when estimating the model parameters (Qian et al., 2005).

2.4.4 Bayesian modelling

As a subset of statistical modelling approaches, Bayesian statistical inference models can exploit disparate sources of environmental information, accommodating natural processes at varying spatio-temporal scales. They decompose the complex and poorly understood interactions in the observed data into a series of conditional likelihood models associated with simple probability relationships, following Bayes' theorem (Bernardo & Smith, 1994; Gelman et al., 2013; Lee, 2016). More specifically, if there are three random variables A, B and C, a factorisation can be written as [A, B, C] = [A|B,C][B|C][C], where [C] denotes the probability distribution of C and [B|C] is the conditional distribution of B given C) (Wikle, 2003b). Normally, it is challenging to describe complicated processes in a spatiotemporal context. However, it is relatively simple to describe the observations in a way that recognises ambiguity due to sampling schemes and inadequate data, as well as the consequent uncertainty. The Bayesian statistical model can be written in three stages (following Bayes' theorem in Equation 2-4): (1) the data model specifies the distribution of observations conditional on the processes and the parameters; (2) the process model describes the underlying processes in the environmental system conditional on the parameters; and (3) the parameter model specifies the distributions for the parameters (Gelman & Hill, 2007; Wan et al., 2014a). The fundamental equation is as follows:

$$\begin{aligned}[process, parameters \mid data] \propto\ & [data \mid process, parameters] \\ & \times [process \mid parameters][parameters]\end{aligned} \quad \text{Equation 2-4}$$

Equation 2-4 integrates the sub-models with the observations and account for different sources of uncertainties. The inference of this integration is the posterior distribution, obtained by updating the probability estimate of the parameters, conditioning on observations and prior distributions. The prior distributions of parameters that are used for likelihood models have to be specified in the parameter model. It is generally assumed that the distributions of different parameters are independent. It is common to use 'vague priors' (minimally-informative) or data-based estimates to define the parameter model when prior information about the parameters is not available. To obtain the posterior distribution of the processes and parameters, a specified sampling technique, such as Markov chain Monte Carlo (MCMC) sampling is used (Gelman et al., 2013).

Bayesian models can be applied to various model structures, and Bayesian hierarchical modelling (BHM) is one of these structures, which has a multi-level structure. BHM has been adopted to understand complex ecological and environmental processes (Berliner, 2003; Gelman & Hill, 2007; Pollice & Jona Lasinio, 2010; Wikle, 2003a, 2003b). The spatio-temporal form of BHM typically includes covariates that vary in time and a semi-parametric spatial covariance structure that represents the complex interrelated nature of multivariate systems (Lee & Newell, 2011; Wan et al., 2014a). The hierarchical model structure allows us to characterise data that are structured in groups (e.g., demographically). Different parameters can be used for each group but sharing information among them constrained by a distribution. In addition, BHM gives uncertainty estimates that could subsequently be considered in decision-making (e.g., water quality management policy) under uncertainties (Rode et al., 2010). This modelling approach also allows an elucidation of the impacts of independent variables at different spatial and temporal scales, on spatially varying regression parameters and parameter distributions (Zhang & Arhonditsis, 2009). More importantly, the separation of data, process and parameter models provides a way of merging physical and statistical modelling, which enables physical reasoning into a hierarchical strategy, as well as quantifies uncertainties arising from data, process and model parameters (Berliner, 2003; Kuhnert, 2017; Wikle et al., 2019).

It is a natural and logical way to build statistical models of the data by decomposing them into several levels (or hierarchy). The posterior distribution is derived by defining the hyperparameters (e.g., parameters of the prior distribution, linking different models describing multi-levels of data), and hyperpriors (i.e., the prior distribution of hyperparameters) (Gelman & Hill, 2007; Gelman et al., 2013). For instance, Zhang and Arhonditsis (2009) developed a conceptual application of the

Bayesian hierarchical framework to allow information to be transferred in space to calibrate a biogeochemical model (Figure 2-5). The bottom level represents the biogeochemical models ($f(\theta_{i,j})$) that estimate pollutant concentrations at individual waterbody i and site j, using parameters $\theta_{i,j}$. At the middle level (i) lake-specific parameter distributions are introduced to estimate spatial variability in the processes within the lake, and the model parameters $\theta_{i,j}$ for a specific lake are drawn from a local population. For the upper level, the lake-specific population parameter mean (μ_i) and variance (σ_i^2) is specified probabilistically in terms of hyperparameters with mean μ and variance σ^2 that represent the entire study area. An advantage of BHM is that it provides a natural structure to reflect situations where each site is different but shares commonalties with other sites in the same system (Rode et al., 2010). This concept allows information to be shared across different locations, which is appealing when dealing with different levels of water quality variations (i.e., spatial and temporal components, see Section 2.2).

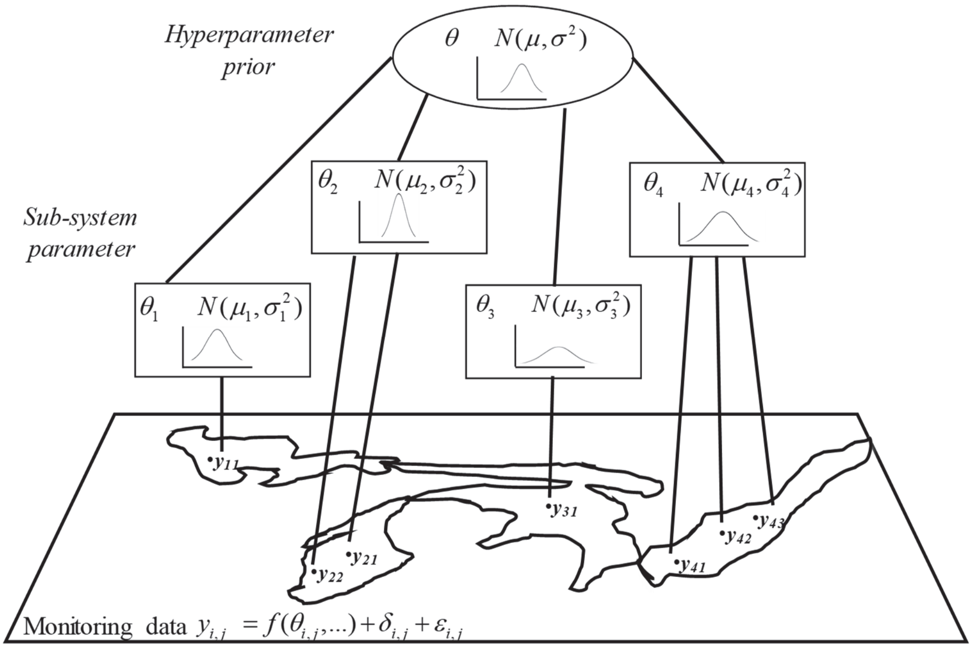

Figure 2-5. A conceptual application of Bayesian hierarchical modelling (BHM). Modified from Zhang and Arhonditsis (2009).

In general, spatial (i.e., site-level mean) and temporal variability (i.e., deviation from site-level mean) in pollutant concentrations was not directly observed generally in the past water quality studies. By using a hierarchical structure, between- and within-sites variability in water quality can be decomposed and investigated separately. The BHM structure has advantages of computational simplicity and flexibility, allowing a framework for combining and updating information (Gelman, 2006; Wu et al., 2011). While, BHM has been increasingly used in a wide range of environmental modelling studies, there have been a limited number of applications to stream water quality behaviours at large scales at different locations (Gladish et al., 2016). This has been partially due to the complexity of describing spatial and temporal processes, and the variability in pollutant concentrations at different levels (between- and within-sites).

2.5 Knowledge Gaps and Research Questions

Degraded stream water quality resulting from elevated levels of non-point source pollutants (Section 2.3) poses significant ecological and environmental threats to the Great Barrier Reef. Previous literature has suggested that spatial heterogeneity in catchment landscapes, such as land cover, climate and geology, has significant impacts on spatial differences in riverine water quality (Section 2.2.1). However, the relative importance of these catchment landscape characteristics has not been well-understood because of the large area of the GBR catchments, limited availability of historical data and other resources required to quantify or model these effects. Understanding the influences of these catchment characteristics on water quality could be very useful for developing management strategies to reduce pollution. Previous studies have not explored the spatial and temporal variation in a systematic manner, which hinders our understanding of key factors affecting each component of water quality responses. Therefore, in this thesis, the spatial and temporal aspects of water quality responses are decomposed and investigated separately. The availability of long-term monitoring data from the Paddock to Reef Program (detailed in Section 3.3) can support the improvement of this understanding using data-driven approaches. This provides an opportunity to further our understanding of the influences of these catchment characteristics on water quality. Thus, the research questions (RQs) of this thesis are:

RQ1: How strong is the spatial pattern of the concentration of water quality constituents across the Great Barrier Reef catchments? Are there groups of constituents with similar spatial behaviour? To what degree is the pattern in water quality associated with the catchment characteristics?

Little research attention has been given to the investigation of key controls on spatial variability in concentrations. Thus, RQ1 explores the underlying spatial pattern of multi-site and multi-parameter water quality constituents, providing an overview of water quality spatial pattern and its association with catchment landscape characteristics.

RQ2: What are the influential catchment characteristics affecting the spatial variability in different water quality constituents? Can we develop a robust statistical modelling approach to predict average water quality responses, using the key catchment characteristics?

While statistical models have shown limited performance when applied to other catchments or time periods, complex process-based models require large amounts of spatial data and long-term continuous water quality and quantity observations for model parameterization, calibration and validation. Hybrid models have been more suitable for large catchments with sufficient number of sites. In addition, model selection uncertainty has remained a problem for traditional regression models when there are multiple competing models that have similar predictive power. Therefore, RQ2 aims to develop a multi-model statistical predictive framework which can address: 1) identification of key factors affecting spatial variation in water quality; and 2) prediction of spatial variability in water quality considering model selection uncertainty.

RQ3: What are the key environmental factors affecting temporal variability in different water quality constituents?

Finally, RQ3 aims to better understand the influential factors affecting temporal variability in water quality and to predict it across multiple locations simultaneously, as well as to address the model selection uncertainty issue in the traditional statistical models. The complex interactions between hydrology, catchment characteristics, and water quality dynamics suggest that modelling of the water quality at all locations individually cannot always be expected. Considering the question as a joint probability problem, aggregating statistical properties (e.g., distributions) over large spatial and temporal scales would be a potential solution. A Bayesian hierarchical framework (BHM, detail in Section 2.4.4) was used in this study to achieve this goal.

In addition to answering the three specific research questions, this thesis contributes to the understanding of water quality dynamics and water quality modelling more generally. Specifically, it furthers the understanding of:

- the spatial and temporal controls on water quality across semi-arid to humid tropical climates;
- the applicability of BHM techniques for spatial and temporal water quality modelling; and
- the uncertainty arising from model selection in statistical modelling of water quality.

Chapter 3 Method and Study Area

3.1 Overview

This chapter begins with a conceptual framework of the entire research, and the methodology (see Section 3.2), followed by an introduction of the case study area and datasets used (see Section 3.3) to address the research questions. This research consists of two major components. Separately, these aim to improve the understanding and predictive modelling of: 1) the spatial variation in stream water quality and 2) the temporal variation in water quality. Detailed descriptions of the methods, study area and datasets used are presented in Chapters 4, 5 and 6, which address individual aspects of the overall study.

3.2 Research Design and Methods

In the previous chapter, three research questions are proposed related to better understanding spatial and temporal changes in water quality and the key drivers of these changes. To bridge the current limitations in statistical water quality modelling identified in Chapter 2, the aims of this thesis were: 1) to associate multi-parameter water quality data from multiple sites with catchment landscape characteristics of these sites; 2) to identify the key catchment landscape characteristics and environmental variables affecting the spatial and temporal variation in water quality; and 3) to quantify the uncertainty associated with predictions (e.g., measurements, model parameters and model selection uncertainty) using data-driven statistical approaches. These considerations lead to the overall conceptual framework used in this thesis (Figure 3-1) and to the methods associated with each research question.

Water quality monitoring data were obtained from the Paddock to Reef Program for the 32 GBR catchments (more details are in Sections 3.3.1 and 3.3.2). This event-based water quality monitoring scheme enabled the investigation of water quality dynamics for runoff events. Considering the complex structure of water quality monitoring datasets (e.g., multiple water quality constituent data collected from multiple locations), multivariate data analyses were used to address RQ1 (Figure 3-1) (Al-Mutairi et al., 2014; Zhang et al., 2019). Specifically, cluster analysis (CA) (Li et al., 2019; Shrestha & Kazama, 2007; Simeonov et al., 2003) , and principal component analysis (PCA) (Gamble & Babbar-Sebens, 2012; Ouyang et al., 2006) were applied to identify the trends in water quality and possible causes of spatial and temporal variability in stream water quality. The implementation of these techniques is detailed in Chapter 4, from which was obtained the key spatial patterns in stream water quality and catchment characteristics, and established links between pollutant source, mobilisation and delivery with catchment landscape characteristics (e.g. land uses).

To address RQs 2 and 3, the total variation in stream water quality was decomposed into spatial and temporal aspects and investigated separately. Given that the statistical data-driven approaches used are subject to uncertainty arising from model selections (i.e., model structures), multi-model inference was adopted as a potential solution to quantifying model selection uncertainty (Anderson & Burnham, 2004; Claeskens & Hjort, 2008; Ye et al., 2008). Application of multi-model inferences can be found in studies in ecology (Hooten & Hobbs, 2015; Johnson & Omland, 2004), groundwater hydrology (Chen & Ma, 2006; Mohan et al., 2018; Poeter & Anderson, 2005; Ye et al., 2010), surface hydrology (Saft et al., 2016), flood forecasting (Abrahart & See, 2002; Duan et al., 2007; Jiang et al., 2018; Wang et al., 2012a), and climate change impact assessment based on global climate models (GCMs) outputs (Cannon, 2015; Deb et al., 2018; Touma et al., 2015).

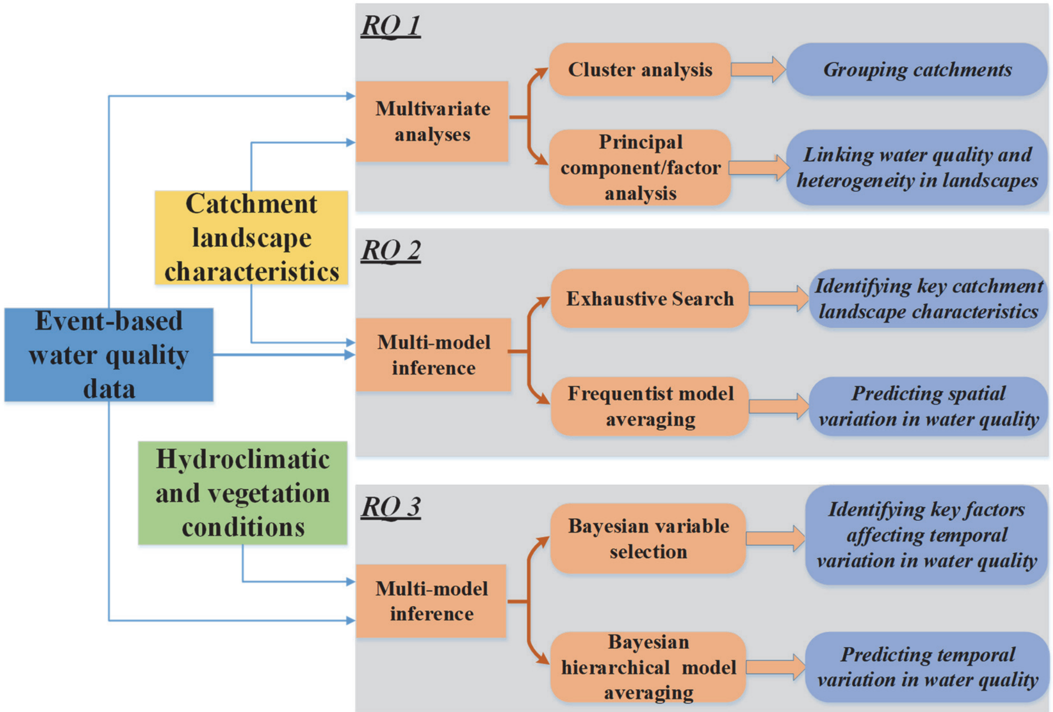

Figure 3-1. The research design of this study.

Both Chapters 5 and 6 describe the detailed development of the modelling framework and evaluation of modelling performance to address RQs 2 and 3. Chapter 5 focuses on analysing the spatial variation of stream water quality (RQ 2) and identifying the key catchment landscape characteristics (e.g., natural and anthropogenic characteristics) that explain these variations (Figure 3-1). A set of plausible models and key catchment characteristics affecting the spatial variation in water quality were identified using an information-based model selection approach and exhaustive search (Burnham & Anderson, 2004). Frequentist multi-model averaging was then used to average predictions across all plausible models to predict the spatial variation in stream water quality.

Chapter 6 addresses RQ 3 (Figure 3-1), which focuses on the temporal variation in stream water quality and the associated influential environmental factors. To jointly address the gaps as outlined in Chapter 2 (e.g., prediction across multiple location and quantification of prediction uncertainties), Bayesian hierarchical modelling and Bayesian model averaging were used to predict water quality temporal dynamics across multiple sites, as well as to quantify the model selection uncertainty. In addition, uncertainties arising from measurements and model parameters can be quantified through Bayesian inference. The integrated modelling framework was able to provide insights into the key environmental factors affecting the temporal changes in water quality and multi-model weighted predictions.

3.3 Case Study Area and Data Sources

A brief description of the GBR catchments, which is the case study area, is presented in Section 3.3.1. This is followed by an explanation of the datasets used in this research (Section 3.3.2 to 0). The water quality sampling data used in this research and the pre-processing method applied to the raw water quality monitoring data is introduced in Section 3.3.2. The candidate spatial (Section 3.3.3) and temporal (Section 0) predictors are then described.

3.3.1 Great Barrier Reef catchments

The Great Barrier Reef (GBR) is the largest natural coral reef ecosystems in the world, covering a sea surface area of approximately 348,000 km^2 and extending over 2,300 km along the northern Queensland continental shelf (Haynes et al., 2007). The adjacent GBR catchments that contribute runoff to the reef have an area of 432,134 km^2 and range from northern to southern coastal and inland Queensland (Waters et al., 2014). There are six natural resource management (NRM) regions, consisting of 35 Australian Water Resources Council (AWRC) basins (Figure 3-2). The characteristics of these NRM regions (in terms of climate, annual rainfall and dominant land uses) are summarised in Table 3-1.

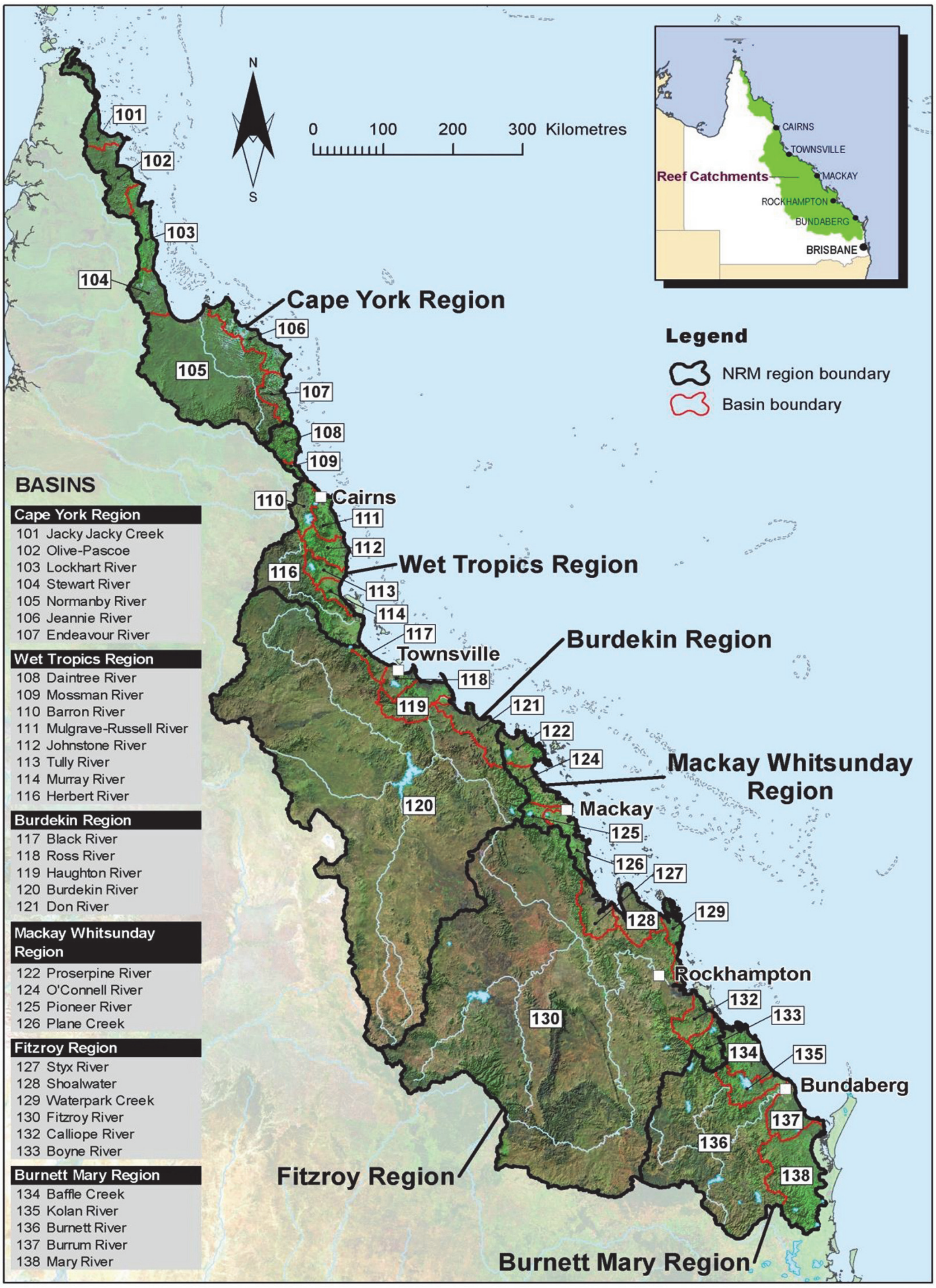

Figure 3-2. The six natural resource management (NRM) regions and 35 Australian Water Resources Council (AWRC) basins making up the GBR catchments. Adapted from Waters et al. (2014).

Table 3-1. Summary of six natural resource management (NRM) regions in the GBR catchments (Waters et al., 2014).

NRM region	Area (km^2)	Climate	Rainfall (mm/year)	Dominant land uses
Cape York	42,988	Tropical with distinct wet and dry seasons	920-2,080	50% Grazing; 48% Forest & nature conservation
Wet Tropics	21,722	Humid tropical	700-4,400	33% Grazing; 51% Forest & nature conservation; 8% Sugarcane
Burdekin	140,671	Dry tropical	500-2,000	90% Grazing; 7% Forest & nature conservation; <1% Sugarcane
Mackay Whitsunday	8,992	Humid, tropical	940-2,000	44% Grazing; 28% Forest & nature conservation; 19% Sugarcane
Fitzroy	155,740	Dry tropical north east to temperate south east	500-1,700	78% Grazing; 14% Forest & nature conservation; 6% Crops
Burnett Mary	53,021	Subtropical	630-1,980	69% Grazing 23% Forest & nature conservation; 2% Crops; 2% Sugarcane

Climate within the GBR catchments varies from tropical to subtropical, with highly variable rainfall across the area. Rainfall is unevenly distributed across the GBR catchments (Figure 3-3). Coastal areas have had the highest mean rainfall (consistently exceeding 3,000 mm/year), which can be attributed to the orographic uplifting effect and the proximity of the oceanic moisture source. Annual average rainfall declines rapidly westward of the crest of the coastal mountain range. The inland catchments of the Fitzroy and Burdekin River basins have mean annual rainfall of only 500-600 mm (Nicholas, 2012).

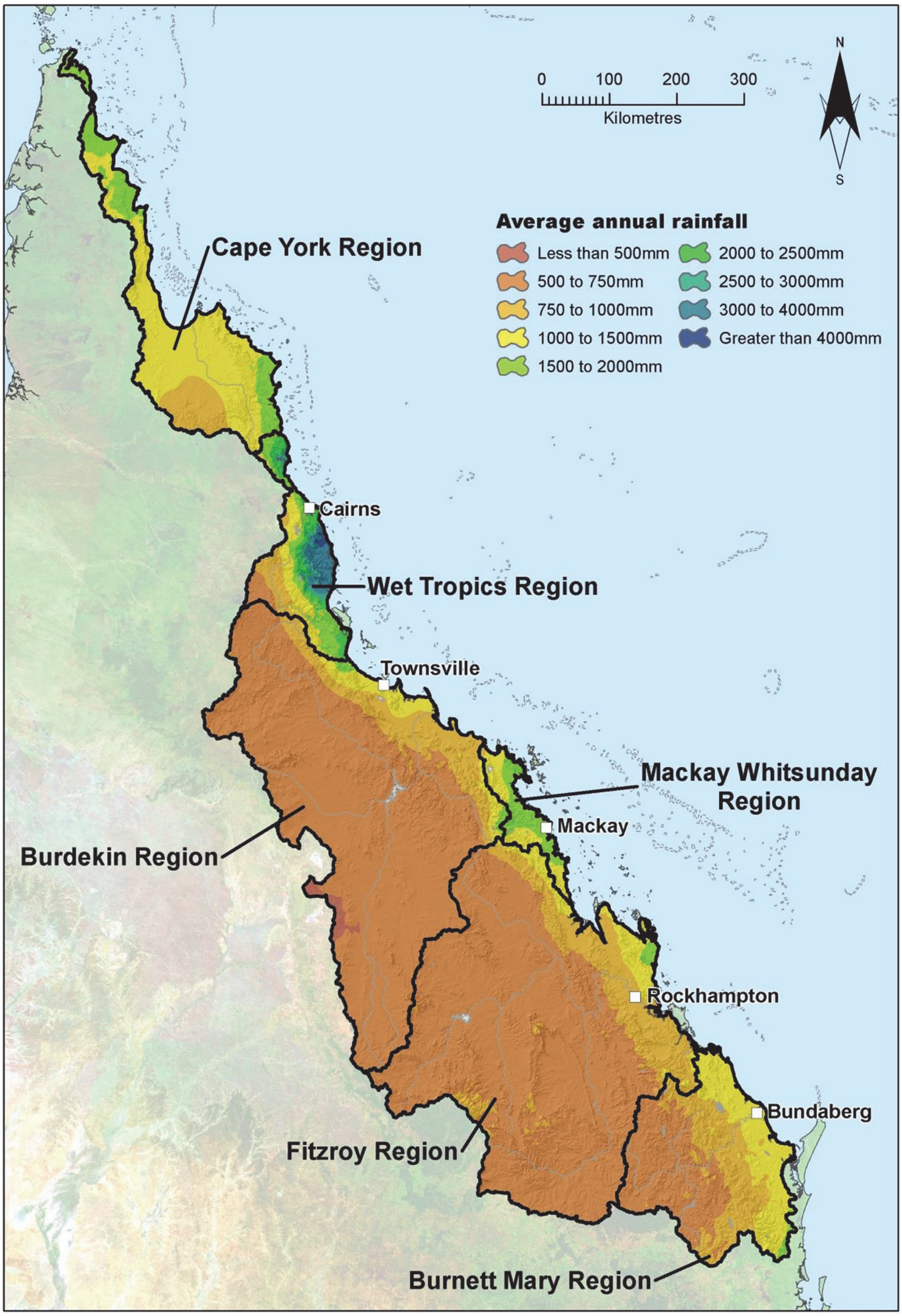

Figure 3-3. Spatial variability in mean annual rainfall across six natural resource management (NRM) regions in the GBR catchments. Adapted from Waters et al. (2014).

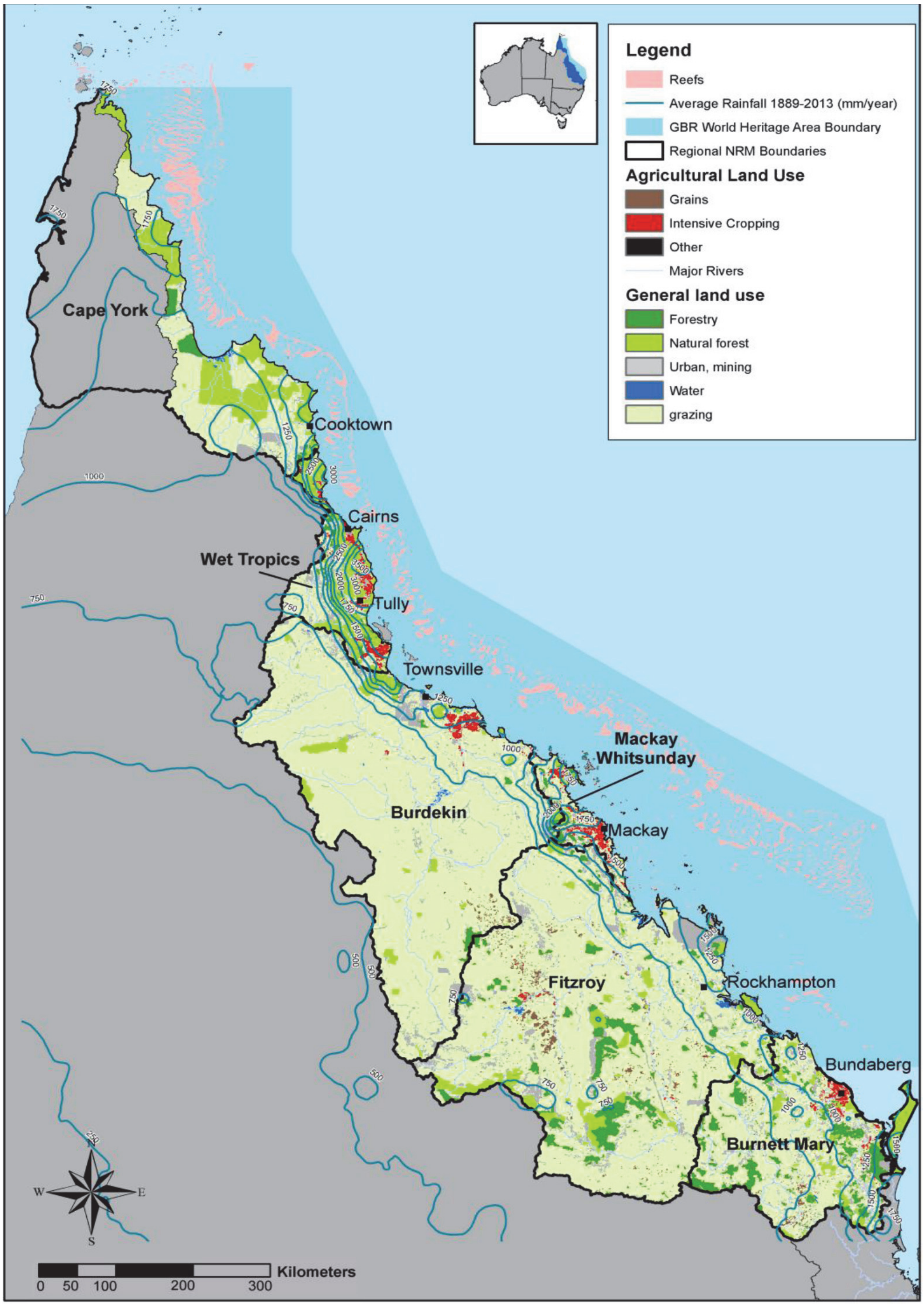

Figure 3-4. Primary land use for the six natural resource management (NRM) regions. Adapted from Thorburn et al. (2013).

The dominant land use in the GBR catchments is cattle grazing (75%), especially in the large and dry inland catchments. Other major land uses include nature conservation (13%) and forestry (5.1%). Cropping consists of approximately 3% of the GBR catchments, almost have of which (1.3%) is sugarcane (Figure 3-4). Due to their higher rainfall, coastal areas (Cape York, Wet Tropics and Mackay Whitsunday) have denser settlements and intensive agricultural land uses (e.g., sugarcane and banana) have developed in the coastal catchments.

3.3.2 Water quality monitoring data

Developing an understanding of region-specific water quality dynamics and water quality modelling relies on water quality monitoring data. The evaluation of water quality observations can also provide valuable information on the long-term trends in water quality (Chang, 2008) and information on important processes affecting water quality dynamics at different spatial scales (Bartram & Ballance, 1996; Mainali & Chang, 2018). In practice, the type and availability of water quality monitoring data has depended on the monitoring objectives and budget (Strobl & Robillard, 2008). In most places, including for the GBR catchments, water quality monitoring programs have consisted of low-frequency, often monthly, grab samples (Behmel et al., 2016; Dupas et al., 2019). However, a key limitation of a low-frequency water quality monitoring strategy is the lack of information obtained on water quality dynamics during runoff/storm events. This is problematic because events typically account for a large proportion of nutrient and sediment loads transported to receiving waters (Lloyd et al., 2016; Sherriff et al., 2015). It is particularly the case for the GBR catchments, where intense runoff over short periods responsible for a large fraction of annual loads of sediments and nutrients (Packett et al., 2009).

With the aim of reducing water quality related risks to the GBR, the Paddock to Reef Integrated Monitoring, Modelling and Reporting Program (Paddock to Reef Program) was implemented in 2006 across multiple GBR catchments (Turner et al., 2012). This program provides improved understanding of annual pollutant loads and good estimates in the reduction of those loads over time. As part of this, a further aim of the Paddock to Reef program is to better quantify the effectiveness of improved land management practices as they are implemented. Given the importance of events for annual loads, event-based water quality monitoring has been undertaken through the Great Barrier Reef Catchment Loads Monitoring Program (Huggins et al., 2018). The resulting water quality monitoring dataset contains both the intensive samples (e.g. daily or every few hours by automatic samplers) taken during the runoff events, as well as grab samples (e.g. monthly) taken under baseflow conditions. The collection of both datasets has enabled reliable calculation of annual pollutant loads (Orr et al., 2014; Waters et al., 2013; Waters & Packett, 2007).

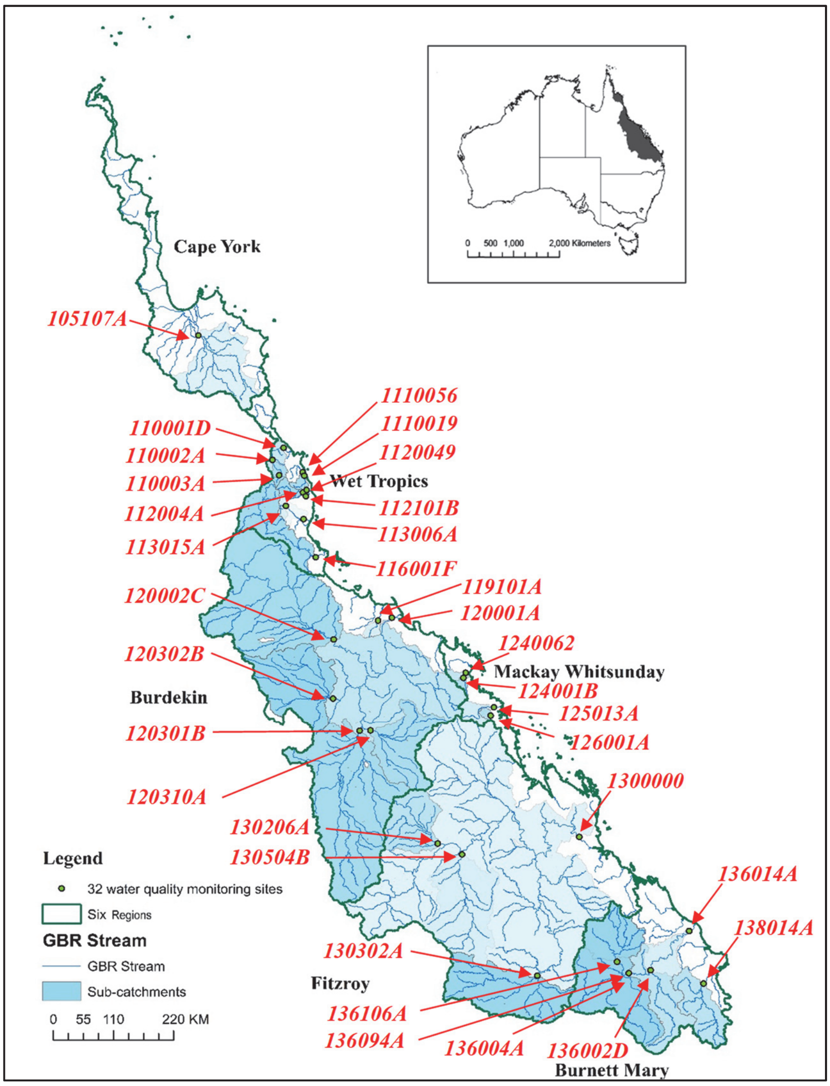

Figure 3-5. Locations of the 32 GBR catchments and water quality monitoring sites in this research.

Nine water quality constituents (total suspended solids (TSS), particulate nitrogen (PN), oxidized nitrogen (NO_X), ammonium nitrogen (NH_4), dissolved organic nitrogen (DON), filterable reactive phosphorus (FRP), dissolved organic phosphorus (DOP), particulate phosphorus (PP) and electrical conductivity (EC)), were included in this research (summarised in Table 4-1, Section 4.3.2). Water quality monitoring data for these nine constituents were collected for the 32 GBR catchments (monitoring sites in Figure 3-5, and more details can be found in Figure 4-1, Figure S-1 and Table S-1) between 2006 and 2016. Figure 3-6 shows a typical TSS monitoring record in one GBR catchment (130000 Rockhampton, Fitzroy River), where more-frequent (e.g. sub-daily) samples were taken during runoff events (e.g., dense red dots over high discharge period in Figure 3-6).

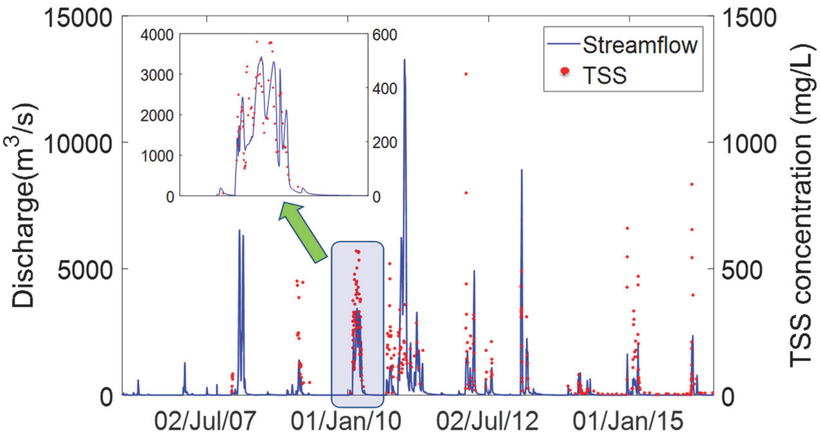

Figure 3-6. Discharge and TSS at 1300000 Rockhampton (Fitzroy River) in the GBR catchments; discharge was measured every 15 minutes.

Event-based sampling resulted in a data set with sporadic bursts of high frequency samples that were interdependent in time. To better characterise the water quality dynamics between runoff events, the event mean concentration (EMC) was calculated as the basis for the statistical analyses and modelling of water quality dynamics in Chapter 5 and Chapter 6. This involved: 1) the delineation of runoff events based on continuous discharge (Figure 3-7 [a]); and 2) the calculation of EMC using the flow-weighted method (Figure 3-7 [b]).

To separate the record into events, an automated runoff delineation method was selected to identify individual events. There are several ways to develop EMCs using water quality monitoring data, depending on the definition of mean concentration over an event and the availability of continuous discharge observations (Bartley et al., 2012). In addition, the flow duration curve can be used to separate water quality samples into ‘dry’ and ‘event’ conditions, and flow events were defined as periods where the discharge was in the highest 5% of flows (Chiew & Scanlon, 2002). They then arithmetically averaged all event water quality samples to obtain their "event mean concentration" (EMC) for a specific catchment. These methods aimed to calculate the 'mean' concentrations that were derived from direct measurements of concentration rather than using the concentration record to derive a load. Others have calculated EMC for individual events. Typically, this involves calculating a flow-weighted or flow and time-weighted concentration, which is essentially the constituent load during each identified runoff event divided by the corresponding event flow volume (Bartley et al., 2012; Johnes, 2007; Marsh & Waters, 2009).

In this research EMCs were calculated for individual events. Event load was estimated by using a flow and time weighted averaging approach, since the concentration samples were well spread over the hydrograph but collected at variable time intervals. EMCs were estimated for events with at least two samples on the rising limb and two on the falling limb (Figure 3-6 and Figure 3-7 [a]), as described in detail in Section 5.3.2.2 (Joo et al., 2012; Waters & Packett, 2007).

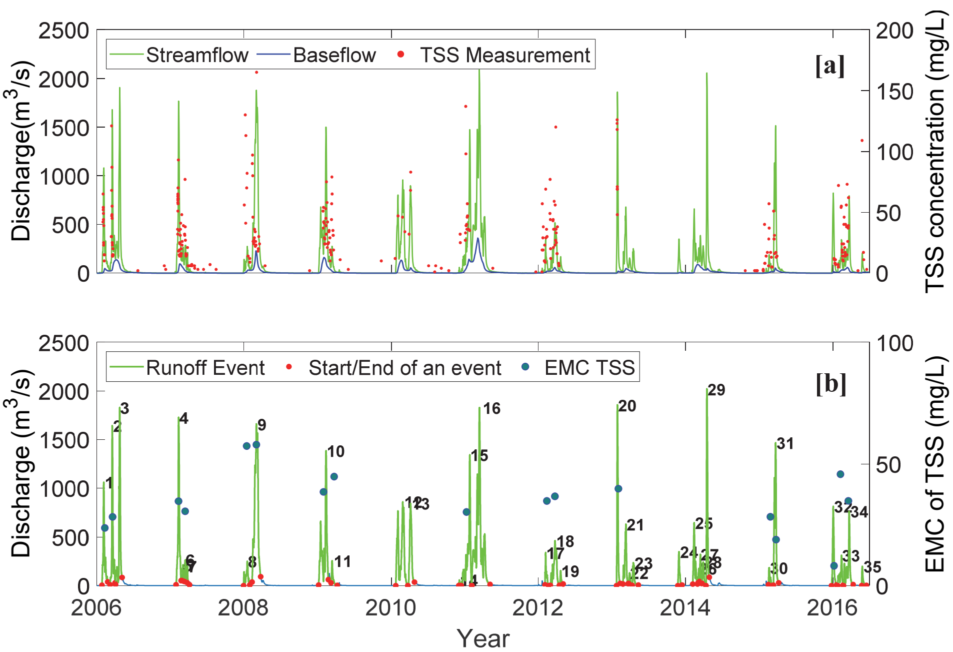

Figure 3-7. Delineation of runoff events and estimation of EMCs, based on the hydrograph for 105107A Normanby River at Kalpowar Crossing in the GBR catchments: (a) baseflow separation from continuous streamflow observations, (b) event identification and development of EMC, and 35 runoff events are identified with red dots representing either the start or end of a runoff event.

3.3.3 Catchment landscape characteristics

To address the RQs 1 and 2, the relationship between spatial variation in water quality and catchment landscape characteristics was investigated. The catchment boundaries of the 32 water quality monitoring sites (Figure 3-5) were delineated using the Geofabric tool provided by the Australian Bureau of Meteorology (BoM) (Bureau of Meteorology, 2012). Through a comprehensive literature review and consultation with catchment managers, fifty-eight different catchment landscape characteristics were collected from publicly available data sets (data sources are in Table S-13). These characteristics spanned six categories; namely, topography, land cover, land use, geology, climate and hydrology. The catchment average values were either extracted by averaging gridded datasets (e.g., catchment average rainfall from BoM) or by calculating the proportion of catchment coverage for polygon datasets (e.g., land use from the Queensland Land Use Mapping Program) (Bureau of Meteorology, 2012; Queensland Government, 2017b). Prior to statistical analyses, these catchment characteristics were transformed to improve data symmetry. More detailed methods are described in Chapters 4 and 5.

3.3.4 Temporal catchment data

Time-varying environmental conditions can influence temporal changes in water quality, and this was investigated to address the RQ 3 (Chapter 6). To achieve this, catchment-averaged hydroclimatic data were used, including runoff, rainfall, air temperature, root zone soil moisture, actual evapotranspiration (AET) and vegetation greenness and coverage. The sources of these datasets can be found in Section 6.3.2.3.

The continuous daily runoff (flow depth in mm) of the 32 catchments was calculated from the daily discharge data obtained from the Queensland Department of Natural Resources, Mines and Energy (DNRME), Water Monitoring Information Portal (WMIP) (https://water-monitoring.information.qld.gov.au/). To visualise the seasonal variation in the catchment average runoff, monthly runoff was calculated and compared for each catchment (Figure 3-8). The distinct wet and dry seasons in the Wet Tropics and Mackay Whitsunday regions is in contrast to the more episodic flows and cease-to-flow periods that were common in the Burdekin and Fitzroy regions. Catchment rainfall and temperature were also extracted from the daily gridded datasets of the Australia Water Availability Project (AWAP) (Raupach et al., 2009). Similar to the monthly runoff, monthly rainfall followed a strong seasonal pattern for all 32 catchments (Figure 3-9), with a large amount of annual rainfall occurring from November/December to February/March the next year. Significant inter-annual variability is evident in both the rainfall and runoff. In addition, catchment root zone soil moisture and AET were extracted from the Australia Landscape Water Balance Model (AWRA-L) (Frost et al., 2016). The ground vegetation condition was summarised by a remotely-sensed vegetation index, the normalized difference vegetation index (NDVI) (Griffith et al., 2002). Specifically, NDVI between 2006 and 2016 was extracted from the Moderate Resolution Imaging Spectroradiometer (MODIS) - MOD13A2v006 (Didan, 2015).

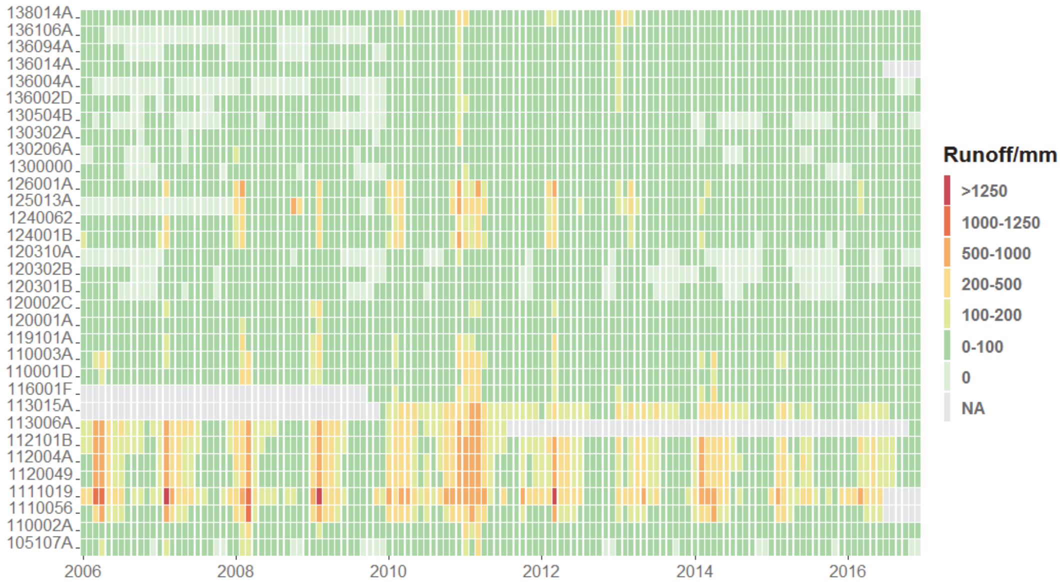

Figure 3-8. Monthly runoff of the 32 GBR catchments in this study from 2006 to 2016; sites id corresponds to the location indicated in Figure 3-5. Sites are ordered from north (bottom) to south (top).

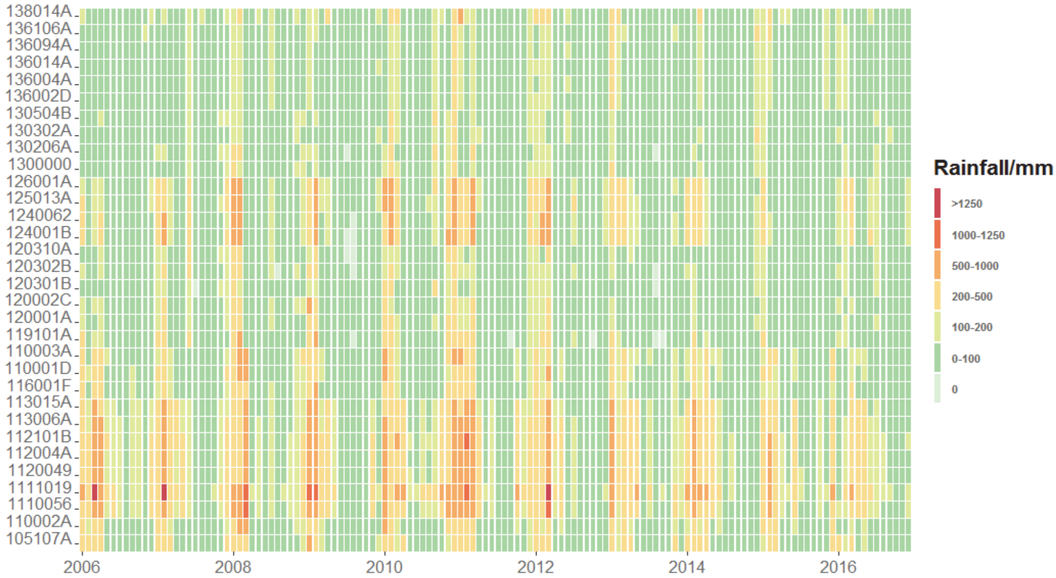

Figure 3-9. Monthly rainfall of the 32 GBR catchments in this study from 2006 to 2016; sites id corresponds to the location indicated in Figure 3-5. Sites are ordered from north (bottom) to south (top).

Chapter 4 Characterisation of Spatial Variability in Water Quality Using Multivariate Statistical Analysis

This chapter was published as the following article:

Liu, S., Ryu, D., Webb, J., Lintern, A., Waters, D., Guo, D., & Western, A. (2018). Characterisation of spatial variability in water quality in the Great Barrier Reef catchments using multivariate statistical analysis. Marine Pollution Bulletin, 137, 137-151. https://doi.org/10.1016/j.marpolbul.2018.10.019

4.1 Abstract

Water quality monitoring is important to assess changes in inland and coastal water quality. The focus of this study was to improve understanding of the spatial component of spatial-temporal water quality dynamics, particularly the spatial variability in water quality and the association between this spatial variability and catchment characteristics. A dataset of nine water quality constituents collected from 32 monitoring sites over a 11-year period (2006 - 2016), across the Great Barrier Reef catchments (Queensland, Australia), were evaluated by multivariate techniques. Two clusters were identified, which were strongly associated with catchment characteristics. A two-step Principal Component Analysis/Factor Analysis revealed four groupings of constituents with similar spatial pattern and allowed the key catchment characteristics affecting water quality to be determined. These findings provide a more nuanced view of spatial variations in water quality compared with previous understanding and an improved basis for water quality management to protect nearshore marine ecosystems.

The key points of this chapter are:

- There is a strong association between spatial pattern in time-averaged water quality and catchment characteristics in the Great Barrier Reef catchments
- Two clusters of sites are identified based on spatial variability in time-averaged water quality.
- Particulate constituents show a strong correlation with grazing land use.
- Oxidised nitrogen shows distinct behaviour in the catchments that might be linked with sugar cane land uses.
- The results add further evidence to support the current overall direction of water quality management in the Great Barrier Reef catchments.

4.2 Introduction

Degradation of water quality is a global issue (Schwarzenbach et al., 2010). Human activities, such as agriculture and urbanisation, are major causes of water quality degradation (Zia et al., 2013). For example, Bricker et al. (2014) showed that the excess nutrient discharge to coastal waters in the Chesapeake Bay region of the USA over the past 200 years was linked to increased anthropogenic pressures, including discharge from sewage treatment plants, and runoff from urban and agricultural land uses.

In-stream surface water quality is important for the health of inland and coastal waters (De'ath et al., 2012; Harris, 2001; Packett et al., 2009). For instance, discharge of sediments and nutrients to marine ecosystems from inland catchments poses a threat to near-shore tropical coral reefs globally (Aronson et al., 2014; Ginsburg & Shinn, 1995). Coral reefs maintain not only environments with rich biodiversity, but they also provide economic benefits from tourism, fishing and aquaculture (Chabanet et al., 1997; Connell, 1978). The ecosystems in the Great Barrier Reef (GBR), Australia, has been deteriorating during recent decades (DeVantier et al., 2006). It is estimated that the GBR-wide coral cover has decreased by 50% since 1985, and the coral cover on inshore reefs has declined by 34% since 2005 (Brodie et al., 2013c). De Valck and Rolfe (2018) estimated that failure to maintain water quality in GBR could result in substantial losses of local economic benefits associated with tourism.

While there are many reasons for the reduction in coral cover in the Great Barrier Reef, poor quality of the water discharging into the reef from the inland catchments is thought to be one major cause (Brodie et al., 2012; Hunter & Walton, 2008; McKergow et al., 2005b). Suspended sediments (often derived from soil erosion) have resulted in a reduction in the light essential for organisms in marine ecosystems, including seagrass and coral. Sediments and organic rich flocculent masses can also smother marine organisms when particles settle out (Brodie et al., 2013c; Haynes, 2001). Nutrients, especially nitrogen and phosphorus, have been closely linked to the observed decline in coral cover through these two mechanisms. Excessive nutrients have facilitated outbreaks of the crown-of-thorns starfish, a major coral predator (Brodie et al., 2005; Fabricius et al., 2010), and they have also been implicated in coral bleaching (Hoegh-Guldberg et al., 2007; Wooldridge & Done, 2009).

To protect aquatic environmental health and values in both rivers and bays, it is recognised that an improved water quality management strategy is essential (Lynam et al., 2010; Santhi et al., 2006; Sidle et al., 2006). This requires a sound understanding of the underlying reasons for water quality degradation in these rivers. However, constituent concentrations are highly variable in space and time due to hydrological variability (Allan et al., 1997b), physical and bio-chemical processes (Ayers & Westcot, 1985; Letterman, 1999; Melching & Flores, 1999) and hydrological transport (Hrachowitz et al., 2016). Therefore, it is important to understand the spatial and temporal controls of water quality (Zhou et al., 2007b).

Previous studies of the Great Barrier Reef catchments using the water quality record have been conducted which either estimated the constituent loads (Kroon et al., 2012; Wallace et al., 2016), or focus on small scale or individual catchments land use effect of pollutant exports (Hunter & Walton, 2008; Lewis et al., 2014; Packett et al., 2009). Other efforts to understand variations in water quality in the Great Barrier Reef catchment have centred on modelling (Carroll et al., 2012; McCloskey et al., 2011; Waters et al., 2013). Through these earlier studies, a conceptual understanding of the role of different catchment characteristics in controlling differences in water quality between catchments is emerging. In addition, given the importance of catchment water quality to the Great Barrier Reef marine ecosystems, a detailed water quality monitoring system has been implemented by the Queensland Department of Science, Information and Innovation (DSITI). The detailed catchment scale monitoring data resulting from that monitoring system has not been systematically compared with catchment characteristics to date.

Most studies addressing the association between water quality and catchment characteristics have focused on temperate catchments in Asia, America and Europe (Ding et al., 2016; Donohue et al., 2006; Lowrance et al., 1997; Renard et al., 1997; Rice et al., 2015; Suif et al., 2016; Vrebos et al., 2017; Wu et al., 2015). Much less research has been undertaken in tropical catchments, like the Great Barrier Reef catchments. The key anthropogenic influences leading to water quality degradation in the Great Barrier Reef catchments have previously been studied at local scales. These include the relationship between sediment and particulate nutrients and erosion processes, and between non-point source dissolved nutrient and pesticide pollution from agricultural activities (Davis et al., 2016, 2017; Kroon et al., 2012; Kroon et al., 2016; McKergow et al., 2005b). These working hypotheses need continual testing as more detailed data emerge.

Multivariate statistical techniques can be used to explore the underlying patterns and potentially the processes affecting multi-site, multi-parameter water quality time-series data. Studies have used multivariate techniques such as cluster analysis and principal component analysis to interpret complex environmental monitoring data (Ouyang et al., 2014; Singh et al., 2004), identify sources of spatial variability in water quality (Mitra et al., 2017; Yang et al., 2010) and assessing monitoring networks (Shrestha & Kazama, 2007; Zhang et al., 2009a). For instance, Li et al. (2011) used cluster analysis to detect the key groups of sites with similar water quality responses along the Middle Route of the South to North Water Transfer Project, China. They identified three groups of sites, reflecting the water quality responses of the sites, reflecting the main drivers of water quality: natural, agricultural and industrial sources.

It is well recognised that spatial and temporal dynamics in water quality are influenced by a wide range of natural and anthropogenic factors (Alberto et al., 2001; Kuhnert et al., 2012; Pratt & Chang, 2012; Singh et al., 2004). In this paper, serving as the initial part of a large study that aims to understand both spatial and temporal responses in water quality, we concentrate on the key catchment characteristics affecting spatial variability in stream water quality. We analysed water quality monitoring data from thirty-two sites using multivariate statistical analysis, over an 11-year period (2006 - 2016), using the time-averaged constituents concentrations (discussed in Section 4.3.4 Data preparation). The aim of the present study was to characterise spatial water quality variation, and to evaluate the relationships between spatial variations in water quality and catchment characteristics (e.g., land use, catchment geological, topographic and climatic conditions). The findings from the Great Barrier Reef catchments contribute to the growing understanding and knowledge of the key factors affecting spatial variability in water quality. In particular, this study addresses the following questions. (i) How strong is the spatial pattern in the concentration of water quality constituents across the Great Barrier Reef catchments? (ii) Are there groups of constituents with similar spatial behaviour? (iii) To what degree is the pattern in water quality associated with the catchment characteristics and what are they? (iv) What is the relative importance of anthropogenic controls and natural controls on water quality, and how these controls inform the management practices to improve water quality? The evaluation of the current conceptual understanding of catchment controls on water quality will further our understanding of spatial controls (e.g., catchment land use and hydrodynamic conditions) of water quality in the Great Barrier Reef catchments, so we can better manage our riverine water quality.

4.3 Materials and Methods

4.3.1 Study area

The Great Barrier Reef catchments are located in north-eastern Australia and encompass northern to southern coastal and inland Queensland. In total, the catchments have an area of 432,134 km^2 and are divided into six natural resource management (NRM) regions (Carroll et al., 2012; Waters et al., 2014) (Figure 4-1). According to the Köppen-Geiger climate classification, the climates in the Great Barrier Reef catchments range from semi-arid tropical or thru warm oceanic to wet tropical (Figure 4-2[a]) (Peel et al., 2007), with annual rainfall ranging from around 500 mm in semi-arid tropical regions to 8,000 mm in parts of the wet tropics where there are strong orographic effects near the coast (Figure 4-2[c]) (Petheram et al., 2008). In most areas, rainfall declines from the coast to inland catchments. Generally, for inland semi-arid tropical regions, the precipitation predominantly occurs during the wet season, from November to April (Davis et al., 2016), while for the costal wet tropics, rainfall is more evenly distributed across the year. Major rainfall events are associated with tropical cyclones occurring in northern part of Great Barrier Reef catchments (Furnas, 2003; Hutchings et al., 2005). Most of the catchments drain eastwards into the Coral Sea from the Great Dividing Range, and they vary widely in topography from rugged mountains to flat river valleys and coastal plains (Figure 4-2[b]).

Land use includes large areas of conservation lands, often covered with tropical forests; and a variety of agricultural uses including pastoral grazing, extensive rain-fed cropping and intensive rain-fed and irrigated sugar cane. Figure 4-2[d] shows that the predominant land uses within the Great Barrier Reef catchments include grazing (~75%), nature conservation (~13%), cropping (e.g., horticulture, ~3%) and sugar cane (~1%) (Queensland Government, 2017a). Denser human settlements and intensive agricultural landscapes have been developed in the coastal catchments. A detailed description of each site in terms of monitored area are provided in Appendix A1, Table S-1.

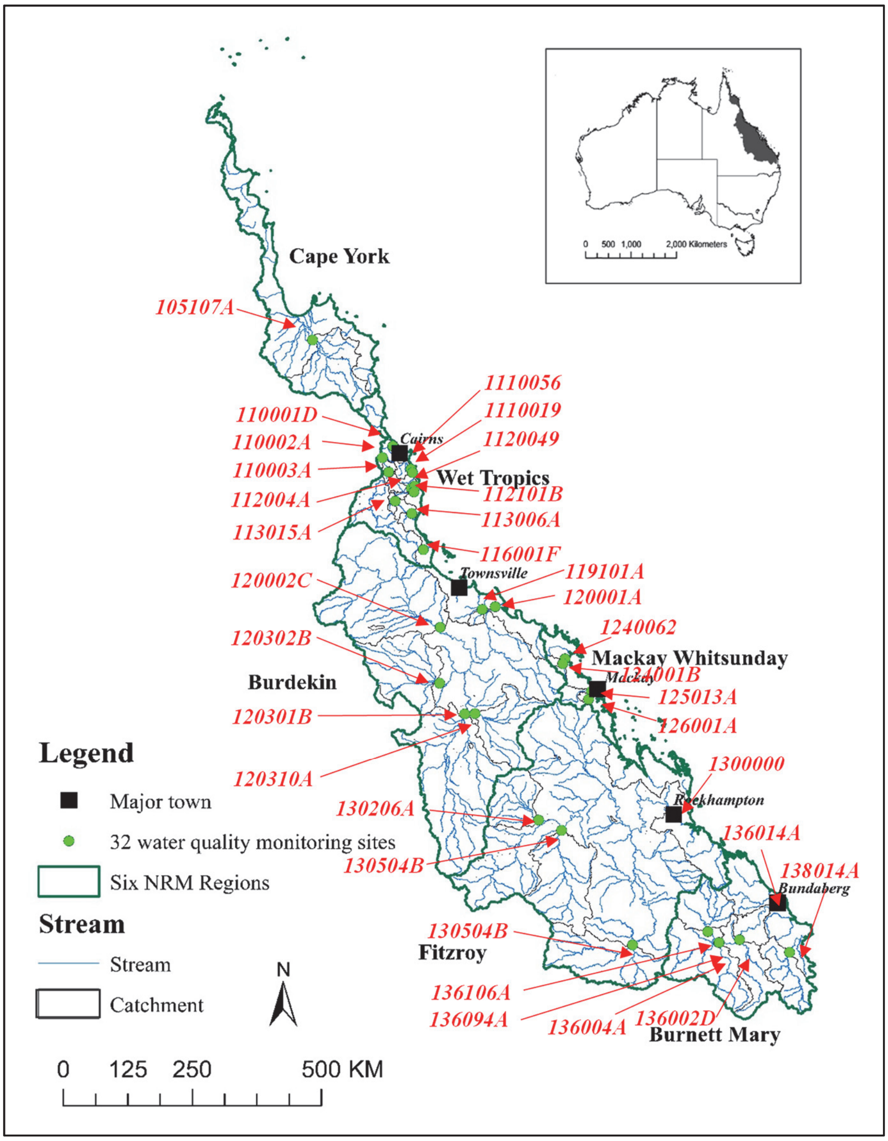

Figure 4-1. Locations of the 32 water quality monitoring sites in the Great Barrier Reef catchments

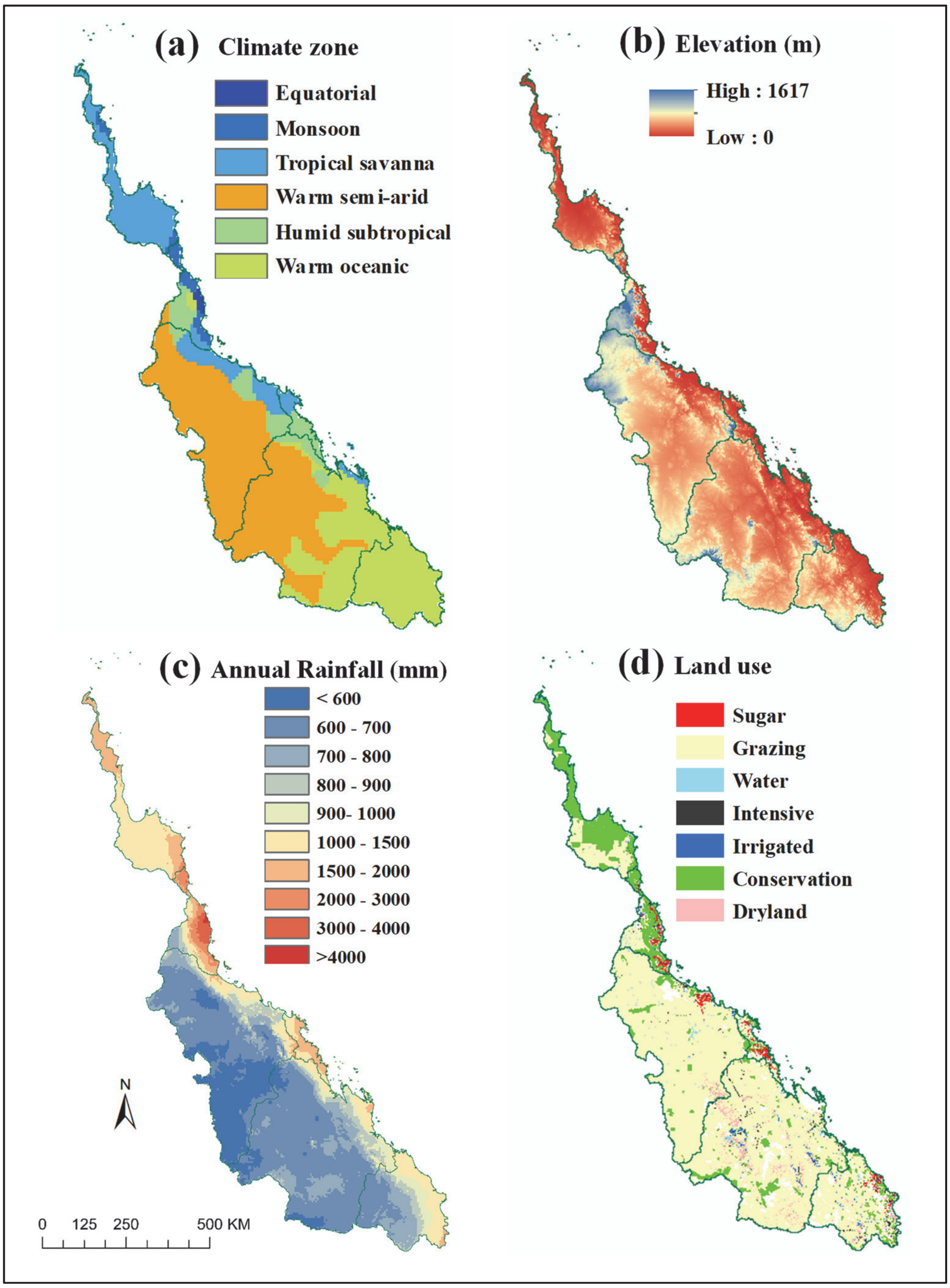

Figure 4-2. Climatic, topographic and land use characteristics across the Great Barrier Reef catchments: (a) Köppen-Geiger climate zone classification; (b) 250 m resolution digital elevation model (DEM); (c) annual rainfall; (d) land use.

4.3.2 Water quality data collection

We used data from 32 water quality monitoring sites (Figure 4-1) across six natural resource management regions. Water quality monitoring data was provided from the Paddock to Reef Integrated Monitoring, Modelling and Reporting Program (Turner et al., 2012). The number of samples and temporal coverage vary by site (Table S-*3*), with largest number of samples were taken at 113006A Tully River at Euramo (e.g., 1441 samples of TSS) between 2006 to 2016 (e.g., 266 samples in 2010, Table S-3). Both intensive event-based water quality sampling during high flow events and monthly sampling during low or base flow (ambient) conditions were undertaken. During event periods, it was common that multiple samples collected on any given day. We analysed data collected from 2006 to 2016. Samples were taken by either manual grab sampling or automatic samplers. The nine constituents considered in this study are summarized in Table 4-1.

Table 4-1**.** Summary information for each monitored constituent (APHA, 2005; Wallace et al., 2016)

Monitored constituents	**Abbreviation**	**Analytical method**	**Practical quantification limit**
Total suspended solid	TSS	Gravimetric	1 mg/L
Particulate nitrogen	PN	High-temperature-combustion oxidation of suspended sediment – Persulfate digestion	0.03 mg/L
Oxidised nitrogen	NO_X	Colorimetric (automated cadmium reduction) method (sum of nitrate and nitrite)	0.001 mg/L
Ammonium nitrogen	NH_4	Colorimetric (automated cadmium reduction)	0.002 mg/L
Dissolved organic nitrogen	DON	Subtracting Particulate nitrogen (PN) ammonium nitrogen (NH_4) and oxidised nitrogen (NO_X) from total nitrogen (TN)	0.03 mg/L
Filterable reactive phosphorus	FRP	Flow Injection Analysis	0.001 mg/L
Dissolved organic phosphorus	DOP	Subtracting filterable reactive phosphorus (FRP) from dissolved Kjeldahl phosphorus (DKP)	0.02 mg/L
Particulate phosphorus	PP	High-temperature-combustion oxidation of suspended sediment – Persulfate digestion	0.02 mg/L
Electrical conductivity	EC	Conductivity probes	1 µS/cm

4.3.3 Catchment characteristics data collection

Previous studies have indicated that catchment characteristics including land use (Li et al., 2009; Uriarte et al., 2011), geology and soil properties (Chang, 2008; Rothwell et al., 2010; Sangani et al., 2015), and climate and hydrology (Kleinman et al., 2004; Smith et al., 1997) can influence the spatial variability in water quality responses (Granger et al., 2010; Lintern et al., 2018a). As such land use, topographic, climatic and soil characteristics were calculated from geospatial data sets for use as explanatory variables in the analysis of spatial variability in water quality responses.

The catchments of the 32 monitoring sites and their corresponding areas were delineated using the Australian Bureau of Meteorology Geofabric dataset (Geoscience Australia, 2011). The characteristics of these 32 catchments varied significantly (Table S-*4* and Table S-5). For instance, catchment annual rainfall ranged from 543.4 to 3744.7 mm. Table 4-2 describes the different types and sources of the catchment characteristics used in this study.

Land use information from the Queensland Land Use Mapping Program (QLUMP) (Queensland Government, 2017a) was used to separate land use into eight categories (Table S-1). A description of how different land uses were aggregated is included in Section A1 in Appendix (Table S-5).

Catchment topographic features (e.g., average slope, stream density and average elevation) and climatic and hydrological attributes (e.g., annual rainfall, temperature and runoff) were retrieved from the National Environmental Stream Attributes dataset (Version 1.1.5) (Geoscience Australia, 2011). Catchment soil erodibility, average soil total nitrogen and clay content were obtained from different geospatial data sets (Australian Soil Resource Information System, 2011; Queensland Government, 2017a; Terrestrial Ecosystem Research Network, 2016).

Table 4-2. Description and data source for catchment characteristics

Catchment characteristics		Unit	Description	Data source
Land use	Conservation	%	Land used primarily for conservation purposes, based on maintaining the essentially natural ecosystems present, such as national park and forest.	Queensland Government (2017)
	Dryland agriculture	%	Land used mainly for primary production based on dryland farming systems (excluding grazing and sugar cane).	
	Irrigated agriculture	%	Land used mostly for primary production based on irrigated farming (excluding grazing and sugar cane).	
	Intensive uses	%	Land subject to extensive modification, generally in association with closer residential settlements, commercial or industrial uses (e.g. urban, utilities, roads).	
	Water	%	Lake, reservoir/dam, river, channel, marsh/wetland.	
	Grazing	%	Grazing native vegetation, grazing modified pastures (native/exotic pasture mosaic, woody fodder plants), grazing irrigated modified pastures.	
	Sugar cane	%	Dryland Cropping (sugar), irrigated cropping (sugar).	
Topography	Slope	°	Catchment average slope.	Bureau of Meteorology (2011)
	Stream density	km/km^2	Ratio of total length of all upstream stream segments to the contributing area.	
	Elevation	m	Average elevation in catchment	
Soil and geology	Soil erodibility	-	Degrees of erosion vulnerability using a limited set of locally relevant soil properties; considers both surface soil stability and subsoil erodibility.	Queensland Government (2017)
	Soil total nitrogen	mg/kg	Average soil TN (in natural N status) content	Terrestrial Ecosystem Research Network (2016)
	Clay	%	0-30cm soil layer clay content	Australian Soil Resource Information System (2011)
Climate and hydrology	Annual rainfall	mm	Average annual rainfall in catchment	Bureau of Meteorology (2011)
	Annual temperature	°C	Average annual temperature in catchment	
	Annual runoff	ML	Average surface runoff in catchment	

4.3.4 Data preparation

The time-averaged constituent concentrations (i.e., average of all available sample concentrations for each constituent at each site) were calculated for each of the water monitoring sites. To justify the use of taking time-averaged constituent concentrations as the spatial representative of water quality response, the sampling distribution relative to the cumulative discharge in each water year (1st July to 30th June) was analysed. The information is further summarised in Figure S-*2*, showing the percentage of samples falling into each 25% of cumulative discharge for each site. Although the samples are not perfectly uniformly distributed across the range of cumulative flow, there is a good coverage of all flow seasons (e.g., early, middle and late seasons) for the majority of sites. Moreover, there is no substantial difference in the distribution of samples across the cumulative discharge curve between the sites (Figure S-*2*), even though there is some variation due to either limited sample numbers or shorter monitoring periods (e.g., 1111019 Russell River at East Russell, 136004A Burnett River at Jones Weir Headwater, 136094A Burnett River at Jones Weir Tailwater and 136106A Burnett River at Eidsvold). Therefore, it is reasonable to assume that the time-averaged concentrations are a good representation of the spatial differences in water quality response.

The time-averaged water quality data were then Box-Cox (Box & Cox, 1964) transformed to improve normality of variables for multivariate statistical analysis (Zhou et al., 2007a). The Box-Cox transformation parameters were different for each constituent. The Box-Cox transformed variables were more normally distributed, with the skewness being close to 0 for most water quality variables (Table S-6).

The log-sinh transformation was applied to all the catchment characteristics, to remove zeros in the raw data (e.g., land use data) (Wang et al., 2012b). Table S-7 (see Section A1 in Appendix) summarises the kurtosis (i.e., a normal distribution has kurtosis exactly 3 (Westfall, 2014)) and skewness of catchment characteristics before and after log-sinh transformation. All the transformed catchment characteristics had an acceptable level of normality, based on p-value (all p-value > 0.01 in Table S-7) of one-sample Kolmogorov-Smirnov test.

4.3.5 Statistical analyses

4.3.5.1 Cluster analysis

Hierarchical cluster analysis was used to test for spatial heterogeneity in constituent concentrations among the monitoring sites in the 32 Great Barrier Reef catchments. For each site, the Box-Cox transformed water quality variable was standardised to have a mean of 0 and standard deviation of 1, to ensure the same scale for all water quality variables. Euclidean distances and Ward's linkage (Singh et al., 2004) algorithm were used in the cluster analyses, which was applied using MATLAB version R2017b (MATLAB and Statistics Toolbox, 2017).

A similar method was also applied to log-sinh transformed catchment characteristics. These data were also standardised before applying cluster analysis. The association of spatial patterns in water quality and catchment characteristics was investigated by checking if clusters derived from the two datasets were similar.

4.3.5.2 Principal component analysis and factor analysis

Principal component analysis and factor analysis are powerful techniques to reduce the complexity derived from high dimensional datasets containing cross-correlated variables (Petersen et al., 2001; Singh et al., 2004). Most studies use the first few principal components (PCs) and rotate these to obtain a new set of factors that can be easily interpreted. This factor analysis further reduces the contribution of less significant variables obtained from a PCA and the new group of variables, known as varifactors (VFs), is extracted (Parinet et al., 2004; Shrestha & Kazama, 2007). The overall aim of this processing is to reduce the number of variables by combining the shared information in closely related variables and to produce more interpretable factors than PCA alone provides. The results in this study were interpreted using the loadings (i.e. coefficients of correlation between water quality/catchment characteristics and VFs) and scores (i.e., representing the relationship between samples and VFs).

We used a two-step PCA/FA on the transformed time-averaged water quality and catchment characteristics separately. The first PCA/FA was solely on the mean water quality constituents at each site. The second PCA/FA was on the catchment characteristics. We used K-means clustering method (see MacQueen (1967) and Hartigan and Wong (1979)) to assess the relationships between two PCA/FA scores, in order to quantitatively evaluate the relevance between features in two lower dimensional subspace (i.e., water quality and catchment characteristics). Several applications (e.g., remote sensing image classification, machine learning and pattern recognition) of PCA together with K-means clustering methods are given in Zha et al. (2002), Ng et al. (2002), Ding and He (2004) and Celik (2009).

Spearman's rank correlation coefficients (Spearman, 2010) between the scores defined by individual VFs from the two PCA/FAs were then calculated, aiming to identify the subset of catchment characteristics that led to the spatial homogeneity/heterogeneity in a group of average water quality responses. Based on the groups from the cluster analysis, we then examined the correlation between VFs scores (i.e., different water quality constituents with similar processes in catchments) in water quality and specific catchment characteristics, to further investigate the key natural and anthropogenic controls on spatial variability.

Similar to the cluster analysis, all the time-averaged transformed mean water quality variables and catchment characteristics were standardised to a mean of 0 and standard deviation of 1, and the analyses (i.e., PCA/FA and K-means clustering) were performed in MATLAB version R2017b (MATLAB and Statistics Toolbox, 2017).

4.4 Results

4.4.1 Cluster analysis

The cluster analyses of both the water quality and catchment characteristics suggested that the 32 sites can be grouped into two clusters (Figure S-3[a] & [b]). There is good agreement between the two cluster analysis results (Figure 4-3).

Specifically, 8 out of the 32 sites are characterised as Cluster one in both analyses (blue round dots in Figure 4-3), and 20 out of 32 sites are identified as Cluster two in both analyses (red triangles in Figure 4-3). The clustering results differ for only 4 sites (blue triangles and red round dots in Figure 4-3). The unusual sites might reflect the substantial contrast in specific land use between catchments. For example, 105107A at Normanby River in the Cape York region has considerable banana cultivation and associated fertiliser application, compared to other catchments (Howley et al., 2013) .This strong agreement between the two cluster analyses indicates that the large-scale water quality spatial pattern is strongly associated with spatial pattern of catchment characteristics. In the following description, the cluster analysis refers to the cluster analysis of water quality responses.

Most of the Cluster one sites are located in the northern region of the Great Barrier Reef catchments. Here, climate (e.g., rainfall in particular), and land use patterns (e.g., fertiliser use on sugar cane) differ from the southern region where most Cluster two sites are situated. Cluster one sites have higher amounts of rainfall (Figure S-5) and more frequent runoff events. In addition, the area of sugar cane proportionally greater in the catchments of these sites (Figure S-4), compared with the southern monitoring sites. Cluster two sites are drier with grazing the strongly dominant land use (Davis et al., 2016).

The median values of average concentrations for Cluster one were lower than those of Cluster two sites except for NO_X (Figure 4-4). All water quality constituents except for NOx and EC, are statistically significantly different between the two clusters (two-sample t-test, $p < 0.05$).

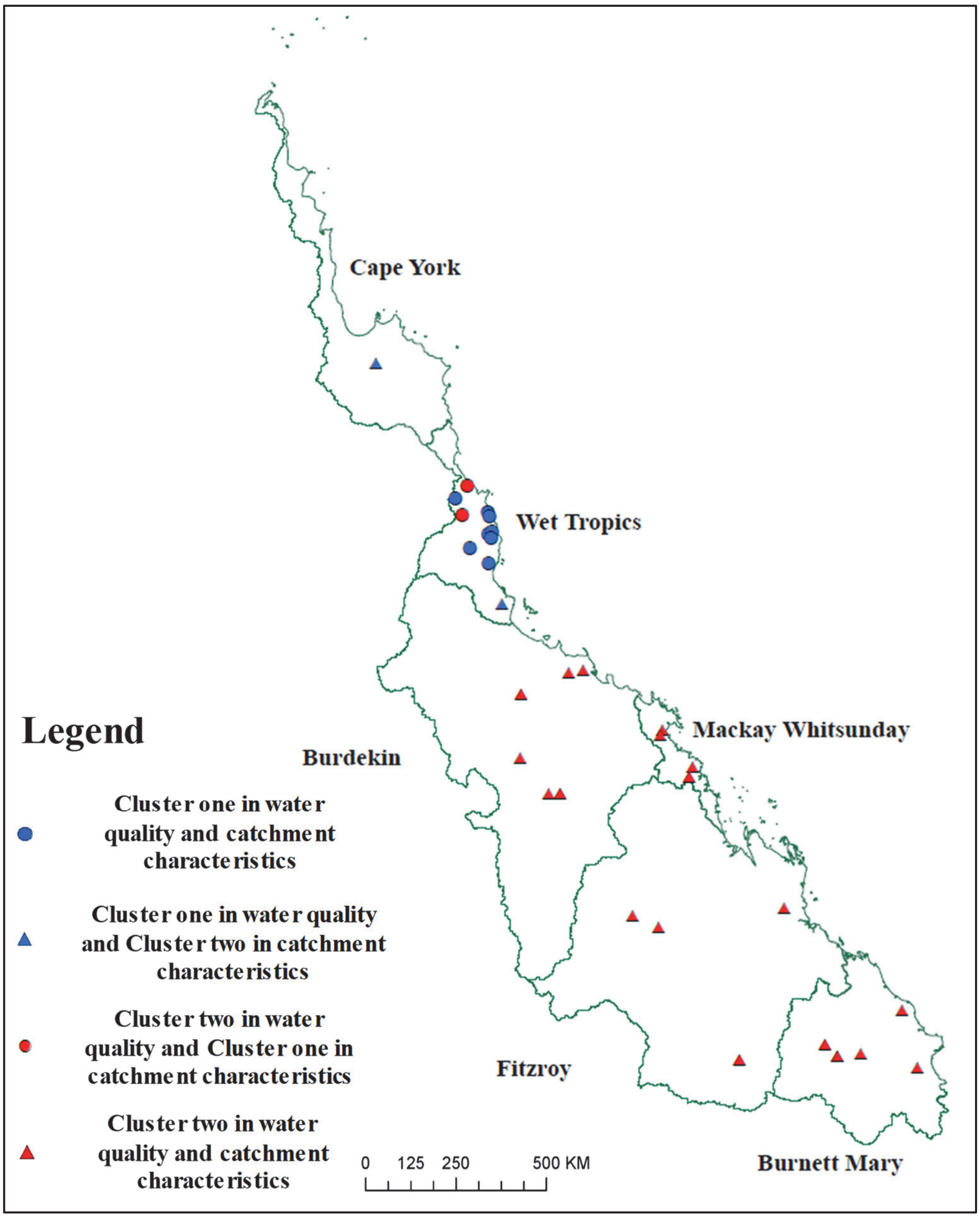

Figure 4-3. Locations of the monitoring sites classified by results of the two cluster analyses. Colour of the markers indicate cluster analysis result of water quality (blue = Cluster one, red = Cluster two). Shape of the markers indicate cluster analysis result of catchment characteristics (round = Cluster one, triangle = Cluster two).

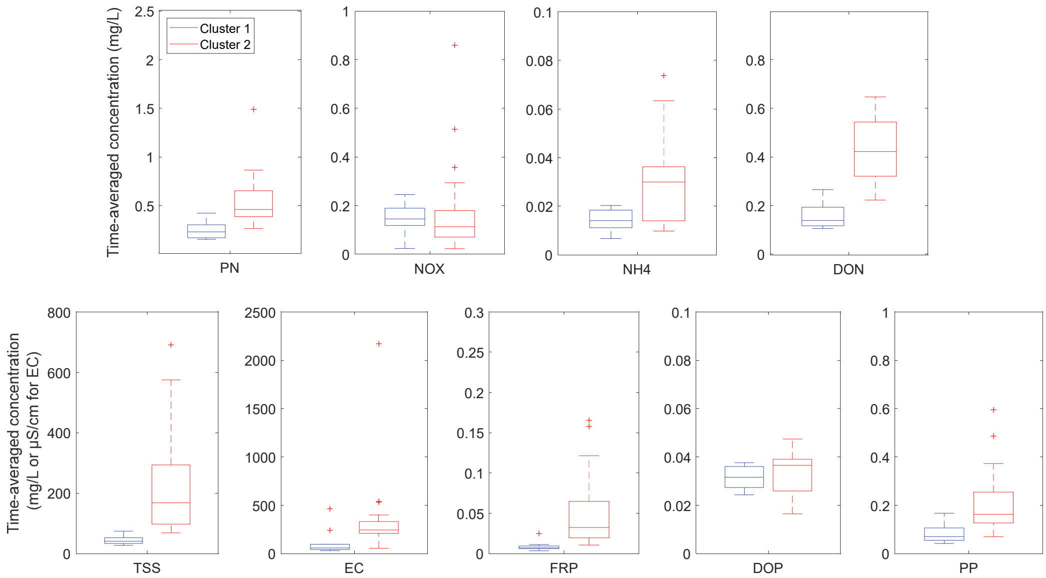

Figure 4-4. Comparisons between the two clusters of time-averaged water quality constituent concentration. The horizontal bars from the top to bottom indicate upper whisker, upper quartile, median, lower quartile and lower whisker, respectively. The plus mark indicates the outliers.

4.4.2 Two-step PCA/FA

4.4.2.1 PCA/FA loadings

The PCA/FA of water quality shows that the first 4 VFs (eigenvalues >1 before rotation), explain 90.7% of the total variance in time-averaged water quality (Table 4-3). In the following discussion, the loadings are classified as 'strong' (absolute loading above 0.75, red in Table 4-3), 'moderate' (absolute loading of 0.5 – 0.75, green) and 'weak' (absolute loading below 0.5, black) (Liu et al., 2003). A second PCA/FA was conducted, in order to link the factors in Table 4-3 to the catchment characteristics (land use, topography, geology, climatic and hydrological data). The first five VFs (eigenvalue > 1) together account for 86.2% of the variance in original data set (Table 4-4).

Table 4-3. Rotated component loadings (varimax) (Abdi, 2003) derived from PCA/FA of mean concentrations of water quality constituents.

Variable	Loading				% Variance explained
	VF1	VF2	VF3	VF4	
TSS	0.94	0.20	-0.12	0.12	94.6
PN	0.94	0.22	-0.01	0.00	93.5
NO_X	-0.03	0.10	0.98	0.06	97.1
NH_4	0.04	0.88	0.33	0.01	88.8
DON	0.48	0.78	0.01	0.12	84.9
FRP	0.66	0.53	0.20	0.31	85.5
DOP	0.12	0.12	0.05	0.98	98.7
PP	0.97	0.09	0.03	0.08	95.2
EC	0.18	0.85	-0.11	0.10	77.5
Eigenvalue	3.42	2.50	1.14	1.10	
% Variance explained	38.0	27.8	12.7	12.2	
% Cumulative	38.0	65.8	78.4	90.7	

Note. VF = varifactor (rotated components using varimax method).
Strong loadings in bold and red; moderate loadings in bold and green.

Table 4-4. Rotated component loading (varimax) derived from PCA/FA of catchment characteristics.

Variable		Loading					% Variance explained
		VF1	VF2	VF3	VF4	VF5	
Land use	Conservation	0.76	0.33	0.03	-0.07	0.49	93.2
	Dryland agriculture	-0.42	0.03	0.48	0.57	-0.09	74.5
	Irrigated agriculture	0.20	0.78	-0.06	0.24	-0.26	78.3
	Intensive uses	0.28	0.84	0.05	0.22	0.02	84.0
	Water	0.68	0.20	-0.58	0.06	0.07	83.0
	Grazing	-0.94	-0.17	-0.06	0.06	-0.05	92.8
	Sugar cane	0.72	0.05	-0.28	-0.21	-0.52	91.6
Topography	Slope	0.94	0.12	0.00	-0.01	0.15	92.2
	Stream density	0.81	0.41	-0.08	-0.29	0.08	92.6
	Mean elevation	0.13	0.70	0.09	0.18	0.45	75.7
Soil and geology	Soil erodibility	-0.40	-0.72	-0.04	0.28	-0.24	81.0
	Mean TN	0.81	0.46	0.22	0.21	0.10	97.4
	Clay	0.25	0.13	0.84	0.21	-0.12	84.5
Climate and hydrology	Annual rainfall	0.93	0.29	0.01	-0.19	0.05	97.9
	Annual temperature	0.07	-0.30	-0.12	-0.85	-0.06	83.0
	Annual runoff	0.27	0.04	-0.39	-0.03	0.75	75.6
Eigenvalue		6.13	3.09	1.58	1.53	1.45	

% Variance Explained	38.3	19.3	9.9	9.6	9.1	
% Cumulative	38.3	57.6	67.5	77.1	86.2	

Note. VF = varifactor (rotated components using varimax method).
Strong loadings in bold and red; moderate loadings in bold and green.

It is useful to examine the key contributors to each VF. VF1 largely represents particulate constituents. VF2 represents most dissolved constituents. VF3 represents NOx. VF4 represents dissolved forms of phosphorus. The picture for the catchment characteristics is less clear due to strong interactions. VF1 (Table 4-4) is strongly dependent on several land uses (conservation, sugar and grazing), topography (slope and stream density), climate (annual rainfall) and soils (nitrogen fertility). High scores on VF1 are for coastal catchments with steep topography, dense stream networks, high rainfalls and relatively high sugar and conservation land uses. Sites with low values of VF1 scores tend to be more inland catchments with opposite characteristics. This illustrates the interactions between climate, topography and chosen land uses. VF2 picks up intensive land uses which tend to also be on less erodible soil. VF3 relates primarily to soil clay content and VF4 to dryland cropping, which correlates negatively with average temperature (Table S-8). VF5 relates to sugar cane, which tends to be in high runoff catchments.

4.4.2.2 Relationships between the PCA/FA scores

To relate the spatial variability in water quality to catchment characteristics, the scores from two the PCA/FA results are investigated. Similar to the result for cluster analysis, the result of K-means clustering analysis of the two reduced dimensional datasets shows that, water quality-based clusters can be reproduced by catchment characteristics-based clusters (an overall 84.4% of matching rate in Table 4-5).

Table 4-5. Classification matrix for K-means clustering analysis of scores from two PCA/FA

Clusters assigned by scores of 5 catchment characteristics VFs	% matching	Clusters assigned by scores of 4 water quality VFs	
		Cluster one	Cluster two
Cluster one	92.3%	12	1
Cluster two	78.9%	4	15
% overall matching	84.4%		

The correlation between scores at each site for different VFs (Table 4-6) shows that most correlation coefficients are low ($\rho < 0.4$), but there are statistically significant pairings. For instance, the scores of ‘Particulate constituents’ VF1 has a negative correlation with the scores on ‘Mixed effect’VF1 in the catchment characteristics ($\rho = -0.61$, $p < 0.01$). Furthermore, Figure S-6 shows that the separation of the two clusters identified in the water quality cluster analysis (red and blue dots) aligns with the variation in the catchment characteristic VF scores (Figure S-6[a]). VF1 in the catchment characteristics PCA/FA results represented the largest variability in catchment characteristics, and most of the Cluster one sites are located in the positive domain, defined by VF1 in catchment characteristics (Figure S-6[a]). While the majority of Cluster two sites are in the negative domain of scores on the VF1 in catchment characteristics.

Figure 4-5 shows the relationships between score on ‘Particulate constituent’ VF1 and specific catchment characteristics identified based on Table 4-4 and Table 4-6. Figure 4-6 shows similar plots for ‘Dissolved nitrogen’ VF2. Together VF1 and VF2 represent the majority of variability (65.8%) in the time-averaged water quality. Spearman’s rank correlation coefficients between scores and catchment characteristics are shown for all sites (black), Cluster one (blue) and Cluster two (red) sites in Figure 4-5 and Figure 4-6. These show that, a stronger relationship is evident between ‘Particulate constituent’ VF1 and catchment characteristics when considering all sites together, while, individual clusters exhibit higher correlations between ‘Dissolved nitrogen’ VF2 scores and catchment characteristics (except for annual runoff Figure 4-6[a]).

Table 4-6. Spearman’s rank correlation between scores on VFs defined by the two PCA/FA.

		PCA/FA for water quality			
		‘Particulate constituents’ VF1	‘Dissolved nitrogen’ VF2	‘NOx’ VF3	‘Dissolved phosphorus’ VF4
PCA/FA for catchment characteristics	‘Mixed effect’ VF1	-0.61**	-0.18	0.43**	-0.21
	‘Intensive uses’ VF2	-0.02	-0.32	-0.02	-0.36*
	‘Soil clay’ VF3	0.12	-0.07	0.05	-0.15
	‘Temperature’ VF4	0.16	0.34	0.14	-0.01

	'Runoff' VF5	-0.08	-0.45**	-0.28	0.05

Note. VF = varifactor (rotated components using varimax method).
* $p < 0.05$.
** $p < 0.01$.

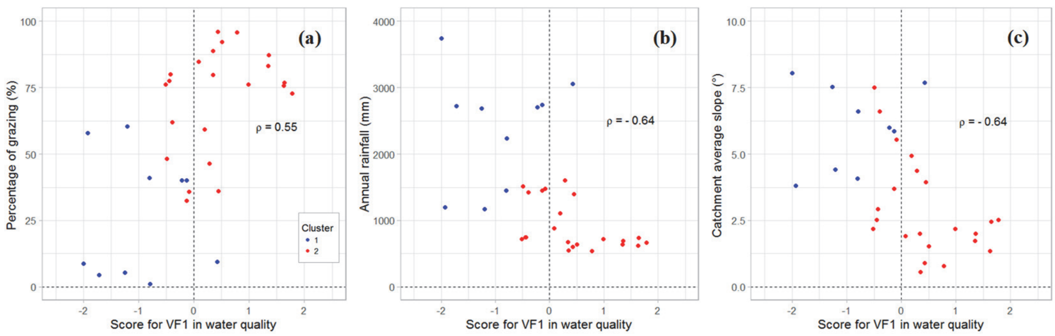

Figure 4-5. Relationship between score on 'Particulate constituent' VF1 in water quality and (a) percentage of grazing, (b) catchment average annual rainfall, (c) catchment average slope. Different colours indicate sites in two clusters: blue = Cluster one and red = Cluster two. ρ indicates the Spearman's rank correlation coefficient.

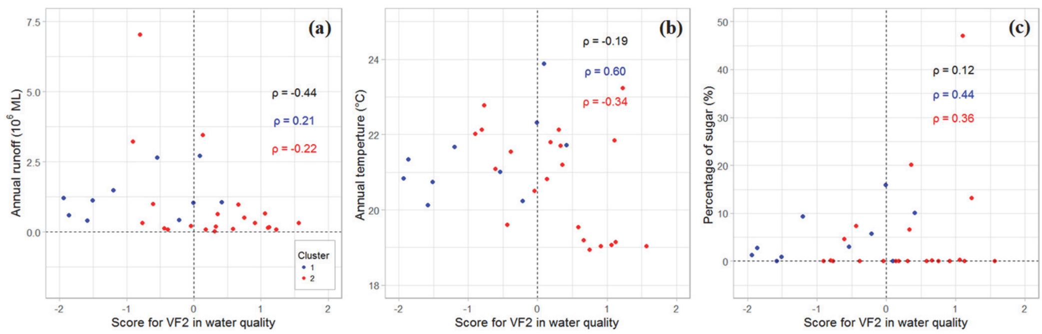

Figure 4-6. Relationship between score on ''Dissolved nitrogen' VF2 in water quality and (a) annual runoff, (b) annual temperature, (c) percentage of sugar cane land use. Different colours indicate sites in two clusters: blue = Cluster one and red = Cluster two. ρ indicates the Spearman's rank correlation coefficient (**note**: black = all sites, blue = Cluster one and red = Cluster two).

4.5 Discussions

4.5.1 Spatial pattern in water quality responses

There are strong patterns in time-averaged water quality responses. Cluster analysis reveals that monitoring sites can be grouped based on similarity in their average water quality for each of the 9 constituents considered (Figure 4-3, Figure 4-4 and Figure S-3[a]). Cluster one sites have lower average concentrations of all constituents except NOx (Figure 4-4), with most of these sites are located in the northern region, where the converse is true for the Cluster two sites. This spatial pattern is evident when evaluating the spatial distribution of VFs scores defined in PCA/FA on water quality (Figure 4-7). Sites with high 'Particulate constituents' VF1 scores (Figure 4-7[a]) are mostly Cluster two sites. The spatial patterns of 'Dissolved nitrogen' VF2 and 'Dissolved phosphorus' VF4 scores are not as evident as VF1, and the average scores of the Cluster two sites for these two VFs are higher than those of Cluster one sites (Table S-10). The 'NOx' VF3 score is higher for the Cluster one sites and several sites in the Fitzroy (Figure 4-7[d]).

The spatial pattern in water quality is strongly linked to catchment characteristics, as the cluster analyses using water quality and catchment characteristics largely agree (Figure 4-3). Cluster one sites are mainly located in coastal catchments in the Wet Tropics region with high annual rainfall and streamflow that is likely to dilute concentrations. These catchments have a mix of conservation, grazing, sugar cane and other intensive land uses (Figure S-4). In contrast, Cluster two sites are dominated by grazing land with small amounts of conservation, sugar and rain-fed extensive cropping. Cluster one sites are much wetter (i.e., higher annual rainfall) than the Cluster two sites. Topography (Figure S-5) tends to show a clear difference between the two clusters (t-test, $p < 0.05$).

VF1 for catchment characteristics is most strongly related to cluster analysis on water quality (Table 4-6 and Figure S-6[a]). This indicates that there is a mix of spatial catchment characteristics controlling spatial variability in water quality. There are both mechanistic links and cross-correlation between catchment characteristics (Table S-8) (Arheimer & Liden, 2000; Lintern et al., 2018a). Further discussion of the association between water quality and catchment characteristics is provided later in the discussion.

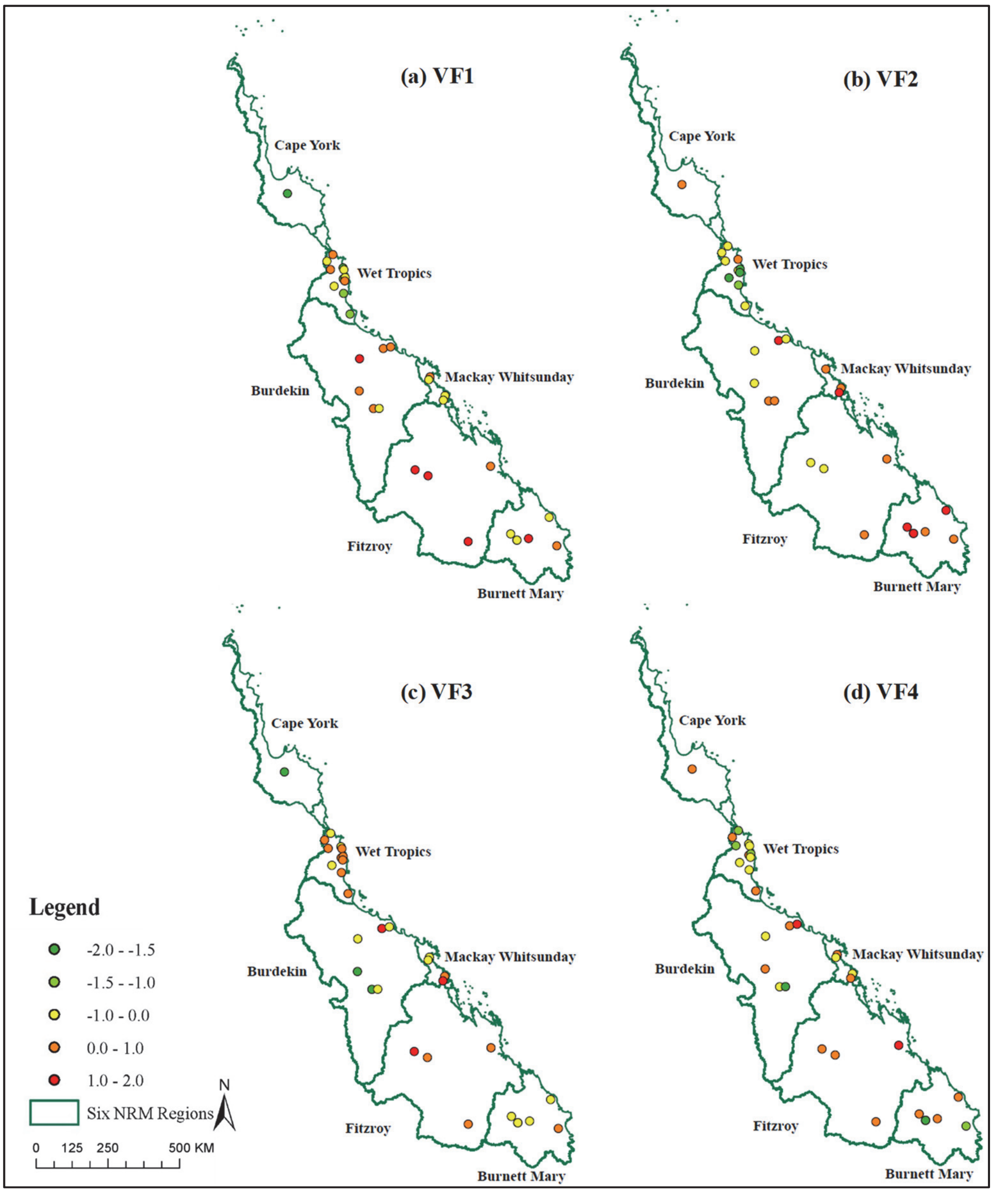

Figure 4-7. Spatial distribution of water quality VF scores: (a) 'Particulate constituents' VF1 score; (b) 'Dissolved nitrogen' VF2 score; (c) 'NOx' VF3 score; (d) 'Dissolved phosphorus' VF4 score.

4.5.2 Groups of constituents with similar time-averaged spatial behaviours

The 9 constituents can be divided into four groups with distinct time-averaged spatial patterns of constituent concentrations according to the PCA/FA analysis (Table 4-3), indicating that there are constituents with common behaviour. The separation of the four groups of constituents indicate that there are systematic differences in the source, processing and/or transport of these constituents compared with the other constituent groups.

VF1, representing the largest proportion of variability (38%), has strong positive loadings on TSS, PN and PP, which are all particulate. Although it is a dissolved compound, FRP has a medium positive loading. This might be caused by in-stream release of inorganic phosphorus from sediments to which they were bound before entering the streams (Gardolinski et al., 2004; Haygarth & Jarvis, 2002). VF2 (27.8% of total variability), has strong positive loadings on dissolved nitrogen (NH_4 and DON, but excluding NO_X), and salinity (EC). This may be associated with hydrological transport processes (Hrachowitz et al., 2016), including discharge between surface water and groundwater for EC, and in-stream biogeochemical processes (e.g., nutrient cycling) for dissolved forms of nitrogen (Dawson et al., 2001; Mulholland & Hill, 1997). VF3 and VF4 explain 12.7% and 12.2% of observed variability in time-averaged water quality, respectively. NO_X and DOP are strongly loaded on these two factors, respectively. The importance of NOx in the results reflects the effect of particular land uses (discussed in Section 4.5.3.3 Oxidised nitrogen).

4.5.3 Examining the association between water quality spatial variability and catchment characteristics

Five factors were identified in the second PCA/FA (Table 4-4) that explain about 86% of the variability in catchment characteristics and that reduce the 16 inter-related catchment characteristics to five independent factors. The characteristics with strong loadings on VF1 (explaining 38.3% of variance) are land uses, topography, and climate and hydrology. The strong cross-correlation between different catchment characteristics (Table S-8) explains these the diversity of catchment characteristics included in this latent factor. For example, flatter, drier more inland catchments are dominated by grazing (slope and grazing: $\rho = -0.89$, $p < 0.01$) and the physiographic characteristics have strongly influenced the land use.

4.5.3.1 Sediments and particulate nutrients

The strong association between 'Particulate constituents' water quality factor and the 'Mixed effect' catchment characteristic factor reveals a combined effect of land use and various physiographic properties on sediments and particulate nutrients, in particular the grazing land use (Table 4-6). Given the range of important characteristics in the 'Mixed effect' factor, there is likely to be multiple factors influencing the spatial variation in sediment concentration. The positive relationship between the percentage of grazing and the score on 'Particulate constituent' VF1 (Figure 4-5[a]) may be explained by the fact that the high proportion of cattle grazing tends to result in a higher rate of soil erosion, leading to an increase suspend sediment sourced from gully, streambank and hillslope erosions (Liu et al., 2017b; McKergow et al., 2005b; Turner et al., 2012). Rainfall erosivity is an important driver of erosion but annual rainfall (and erosivity) is lower in the catchments with higher sediment concentrations (Figure 4-5[b]). In the drier catchments, events are typically separated by long dry periods, resulting in highly ephemeral flow and sporadic runoff events with higher peak sediment concentrations during the 'first-flush' in dry-tropical rivers (Davis et al., 2016; Packett et al., 2009). This counter-intuitive relationship with spatial rainfall and the 'first-flush' effect suggests that lower vegetation cover interacting with rainfall events may be the important influencing processes, rather than rainfall erosivity.

All else being equal, high topographic slope is expected to lead to greater erosion by any surface flows and better delivery to stream, although high slope should also preference subsurface flow over surface flow. Counterintuitively, the data (Figure 4-5[c]) shows a negative relationship between the 'Particulate constituent' VF1 score and catchment slope. This unexpected effect of slope could be explained by the correlations with other catchment characteristics, rather than being a causal factor in the spatial variation of sediment concentrations. For example, most of the flat catchments (Cluster two sites) are inland catchments, where a large proportion of grazing land might act as a source of sediment. This finding is supported by a regional study in Fitzroy River catchment, which found that the high fine sediment concentrations during the event were closely associated with a high percentage of rainfall on cropping (Packett et al., 2009).

4.5.3.2 Dissolved nitrogen and salinity

The ‘Dissolved nitrogen’ score (VF2) correlates with both the ‘Runoff’ (VF5) and ‘Temperature’ (VF4) factors (Table 4-6). Catchment climate and hydroclimatic characteristics, such as annual runoff (Figure 4-6[a]) and annual temperature (Figure 4-6[b]), have considerable contributions to these two VFs. Previous studies showed that these catchment characteristics could influence the mobilisation and transport of dissloved nitrogen and EC (e.g., mineralistaion of organic matter or desorption form particulates, and transportation of EC in the sub-surface flow pathway) (Donnelly et al., 2011; Fritz & Anderson, 2013; Lintern et al., 2018a). Indeed, we found a significant and negative correlation for both mean annual runoff and temperature with DON and NH_4 and EC (Table S-9).

There is a negative correlation between annual runoff and VF2 scores (Figure 4-6[a]), and the difference in the level of the VF2 scores for the two clusters suggests contrasting hydrologic behaviours (e.g., hydrological variability) of the streams. The comparison of flow duration curves (daily flow depth in mm calculated from daily discharge data obtained from the Department of Natural Resources, Mines and Energy, Water Monitoring Information Portal, Figure 4-8[a]) show that the majority of the Cluster one sites (i.e., blue curves in Figure 4-8[a]) feature perennial characteristics with less variability in daily streamflow compared with the Cluster two sites (i.e., red curves in Figure 4-8[a]). The Cluster two sites with higher coefficient of variation of daily flow depth than Cluster one sites (Figure 4-8[b]). This indicates that the perennial Cluster one streams are in areas with higher runoff coefficients and thus more leaching. As a result, dissolved nitrogen and EC could be transported more broadly across the catchment, thus lowering the average concentrations. In contrast, the majority of streams of the Cluster two sites are ephemeral rivers (i.e., red curves in Figure 4-8[a] and red dots in Figure 4-8[b]), and the more variable with longer low flow period may lead to a changing source of surface runoff, by providing more groundwater with high salinity that differs chemically from stream water (Moore et al., 2008).

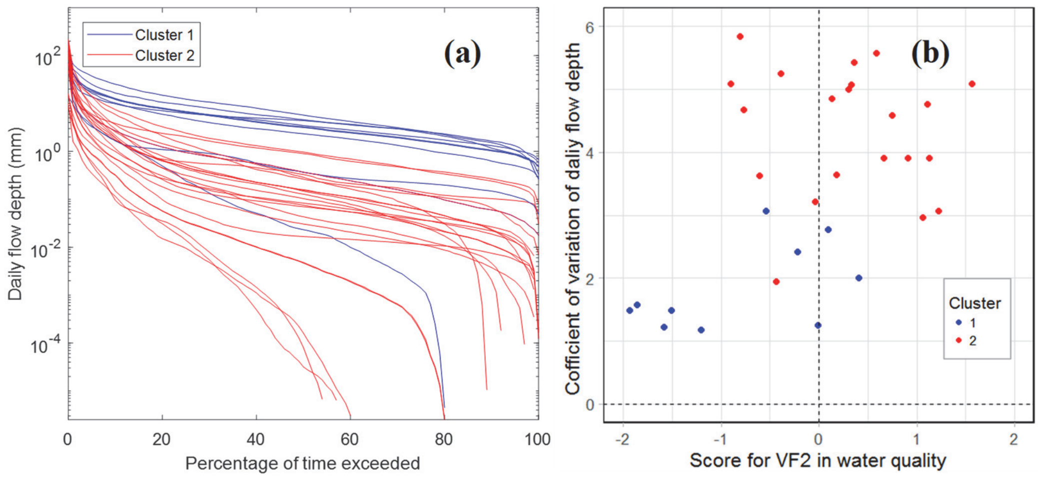

Figure 4-8. Impact of hydrological variability on 'Dissolved nitrogen' VF2, (a) Comparison of flow duration curves of the 32 Great Barrier Reef water quality monitoring sites. (b) Relationship between VF2 scores and coefficient of variation of daily flow depth for each site. (**note**: different colours indicate sites in two clusters: blue = Cluster one and red = Cluster two).

Interestingly, the relationships between scores on 'Dissolved nitrogen' VF2 in water quality and annual temperature (Figure 4-6[b]) differ between the two clusters (significantly different according to 10,000 bootstrap testing on the test statistic - difference in two correlation coefficients, and the 95% confident interval is away from 0). The positive effect of temperature on 'Dissolved nitrogen' VF2 for the Cluster one sites (blue scatters in Figure 4-6[b], $\rho = 0.60$) score is likely due to the cross-correlation between climate and land uses in different catchments. Higher annual temperature favours sugar cane growth, leading to an increase in scores on 'Dissolved nitrogen' VF2 when annual temperature is higher. In contrast, the negative relationship between annual temperature and scores on 'Dissolved nitrogen' VF2 for cluster two sites ($\rho = -0.34$) land use and cover have an impact on dissolved nitrogen in runoff. For example, Brigalow Belt regions (e.g., Fitzroy and Burdekin), where these is a broad-scale inclusion of virgin brigalow woodland into agricultural uses (e.g., pasture legumes), has been identified as a major source of dissolved organic nitrogen (Allen et al., 2016; Elledge & Thornton, 2012, 2017). Sugar cane (Cluster two sites, blue dots in Figure 4-6[c]) where excessive fertiliser might be applied, is another nitrogen contributor associated with NH_4 (Davis et al., 2016). In addition, it is argued that higher temperatures could favour denitrifying bacteria, thus reducing the level of ammonium nitrogen in the catchments (Smith et al., 1997).

4.5.3.3 Oxidised nitrogen

A distinct constituent, NO_X, identified in the final VF in water quality, appears to be linked to 'Mixed effect' VF1 of catchment characteristics PCA/FA (Table 4-6, $\rho = 0.43$). While this is also true of the particulates, the direction of correlation is opposite. Table 4-4 and Table S-9 show that sugar cane followed by stream density and annual rainfall are the three main characteristics positively correlated with the spatial variability in NO_X. This result is not unexpected as Biggs et al. (2013) and Mitchell et al. (2005) have previously shown that for catchments in the Mackay-Whitsunday region, the majority of NO_X losses from the catchment occur via deep drainage and runoff derived coupled with sugar cane plantations, where high nitrogenous fertilisers are applied. Regions such as the Wet Tropics and Mackay-Whitsunday, have a high proportion of sugar cane and horticultural cropping (>8% of the catchment area). This further suggests that nitrogenous fertilisers are an important source of NO_X in these catchments (Azizian et al., 2015; Mitchell et al., 2005; Reddy et al., 1989). The positive correlation between 'Oxidised nitrogen' VF3 score and stream density ($\rho = 0.44$) and annual rainfall ($\rho = 0.38$) indicates that NO_X might be transported where stream networks are well-developed in relatively wet catchments, reducing the residence time of NO_X and thus resulting in a higher riverine oxidised nitrogen concentration (Edwards & Withers, 2008; Liu et al., 2017b).

4.5.3.4 Dissolved phosphorus

Table 4-6 shows that the 'Dissolved organic phosphorus' VF4 score (Table 4-3) is significantly and negatively correlated to 'Intensive uses' VF2 score (Table 4-4) in the second PCA/FA ($\rho = -0.36$). A negative correlation between DOP and these two land use categories (i.e., intensive and irrigated land uses) is also found (Table S-

9).In contrast, other studies (Chantigny, 2003; Kroon et al., 2012; Mattsson et al., 2005; Palviainen et al., 2016) showed that dissolved phosphorus concentration was positively correlated with catchments with a higher proportion of cropping agriculture (non-point source), sewage treatment plants or industrial discharges (point source). The contrasting results might be explained by the scale of monitored catchments in this study being so large that the input of DOP associated with the specific land uses (e.g., source from animal waste) might not be detectable (Hunter & Walton, 2008). In addition, the biogeochemical cycling and associated transport of dissolved phosphorus (e.g., DOP) might lead to the spatial heterogeneity in 'Dissolved organic phosphorus' VF4 score (Figure 4-7[c]) (Robson, 2014; Vadas et al., 2005).

4.5.4 Management practice implications

Over the past decade, the Reef Water Quality Protection Plan (Brodie et al., 2013c) led to the introduction of specific regulations and incentives for the adoption of the improved management practices in the Great Barrier Reef catchments (Waters et al., 2014). Farmer have been encouraged to implement these to minimize the risk of fine sediments and nutrients inputs to the Great Barrier Reef marine ecosystems (Thorburn et al., 2013).

The original water management plan was based on a range of lines evidence that suggested large grazing catchments were targets in reducing sediments (e.g., protection from soil erosion processes) and key management practices were adopted to control DIN exported from sugar cane land use (Lewis et al., 2014; Waters et al., 2014). The monitoring data analysed here were collected to further understand loads and patterns of loads at the catchment-basin scale. Our results are consistent with the current understanding developed at smaller scales that shows land use and management practices are important factors affecting the spatial variability in water quality responses (Brodie et al., 2017b; Hunter & Walton, 2008; Lynam et al., 2010; Thorburn et al., 2013). Grazing land use has a strong association with spatial variation in sediments and particulate nutrients across the Great Barrier Reef catchments, with particulates being identified as a key source of impact on the

Great Barrier Reef aquatic environment. A continued concentration on management of sediments in the large grazing catchments is supported by our results. In addition, there is a strong correlation between the area of sugar cane and dissolved inorganic nitrogen concentrations. Again, our results support continued focus on intensive agriculture, in particular sugar cane, in addressing NO_X impact on the Great Barrier Reef. Finally, catchment topographic characteristics, interacting with land uses, might also influence these different types of constituents. In particular, the results suggest that focusing fertiliser management on catchments with high stream density and annual rainfall (strong hydrologic connectivity) and sugar cane activities might be worth more in-depth investigation to establish, if real benefits could be achieved in reducing dissolved inorganic nitrogen in streams.

Catchment climate and hydrology affect spatial variability in dissolved nitrogen species (except for NO_X) and salinity. This is likely a result of cross-correlation of these catchment characteristics and land uses and catchment geology. We also found that the relationship of the spatial pattern of the main dissolved constituents (e.g., dissolved nitrogen and EC) and catchment characteristics differs for the two clusters of sites across the Great Barrier Reef catchments. A sound understanding of the underlying reasons for the differences in these relationships is necessary for effective water quality management policy-making. Indeed, the hydrological variability, in-stream biogeochemical processes, as well as sources from different land uses are significant factors that can lead to varying behaviours of dissolved nitrogen and EC among two clusters of sites. This implies that there is not a 'one-size-fits-all' approach to managing water quality throughout the whole the Great Barrier Reef catchments. It should also be noted that pesticides have been identified as important water quality parameters in the context of the Great Barrier Reef catchments, but that they are excluded from this study.

4.6 Conclusions

This study applied multivariate statistical techniques to understand the spatial variability in stream water quality in the Great Barrier Reef catchments. We found that different catchment characteristics influenced the magnitude of concentration in varying ways in the Great Barrier Reef catchments. The influences of the key catchment characteristics depended on clusters of sites and their impacts differed for different constituents. Therefore, a comprehensive understanding of spatial variability and its association with catchment characteristics is likely to provide valuable information for catchment management make decisions aiming to address the risks of land-derived constituents on the marine aquatic ecosystems. It is important to note that water quality varies in time, as well as space, and temporal drivers (e.g., discharge, spatial and temporal differences in land use and management and cover, etc.) of water quality variation in these catchments is the subject of ongoing investigation to improve our understanding of water quality dynamics.

Chapter 5 Understanding the Impacts of Catchment Characteristics on Spatial Variability in Water Quality: A Case Study in the Great Barrier Reef Catchments

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5.1 Abstract

Water quality monitoring programs often collect large amounts of data with limited attention given to the assessment of the dominant drivers of spatial and temporal water quality variations at the catchment scale. This study aims to: a) identify the influential catchment characteristics affecting spatial variability in water quality, and b) develop predictive models to estimate average concentration of water quality constituents. Tropical catchments in the Great Barrier Reef area, Australia were used as a case study. Water quality monitoring data (i.e., sediments, nutrients and salinity) from 32 sites together with 58 candidate catchment characteristics were used to construct statistical models. Exhaustive Search method coupled with multi-model inference approaches were adopted to identify important catchment characteristics and predict the spatial variation in water quality across catchments. The results indicate that water quality variables were generally most influenced by the natural characteristics of catchments (e.g., catchment topography, geology and climate), while anthropogenic characteristics (i.e., land use) also showed significant influence on dissolved nitrogen species (e.g. NO_X, NH_4). Not only does this study indicate the key drivers and provide water quality predictions in the tropical Great Barrier Reef catchments, the statistical models could also potentially be used to assess stream water quality changes likely to occur under future climate and land use changes. Therefore, the established models could enable water resources managers to pre-emptively implement appropriate management strategies.

The key points of this chapter are:

- A multi-model approach is used to assess the impacts of catchment landscapes characteristics on the spatial variation in water quality.
- Catchment natural characteristics exhibit most impact on water quality overall, but land use has an important impact on dissolved nutrients.
- The established models and the associated catchment characteristics enable prediction of the spatial variability in catchment water quality.

5.2 Introduction

Fresh water resources are key to agricultural, industrial, and environmental activities (Kundzewicz et al., 2007). However, there is a worldwide concern that water quality in rivers and streams is deteriorating (Booth et al., 2016; Hiscock & Grischek, 2002; Zhao et al., 2019). The elevated levels of pollutants in streams can lead to substantial economic and environmental losses, particularly in coastal and estuarine ecosystems (De Valck & Rolfe, 2018; Pickering & Pottinger, 1987). To address riverine water quality degradation, improved management in many coastal regions has been implemented in recent decades, e.g. Chesapeake Bay in the U.S.A. (Preston & Brakebill, 1999; Zhang & Blomquist, 2018) and the Great Barrier Reef catchments in Australia (Brodie et al., 2017b; Schaffelke et al., 2012; Waterhouse et al., 2017).

The effectiveness of implementation of improved management practices heavily depends on a sound understanding of pollutant processes (i.e. source, mobilisation and delivery) in catchments (Granger et al., 2010). Riverine water quality is highly variable across space and time and is affected by a wide range of natural and anthropogenic factors in catchments (Chang, 2008; Guo et al., 2019b; Lintern et al., 2017; Zhang et al., 2016b). Therefore, it is important to understand the key factors affecting spatial and temporal variability in riverine water quality.

Within a catchment, water quality exhibits substantial temporal variability, including at daily (Brainwood et al., 2004; Meybeck & Moatar, 2012), seasonal (Ouyang et al., 2006; Xiaolong et al., 2010; Xu et al., 2019a) and inter-annual (Fabricius et al., 2013; Zhuo et al., 2016) scales. This variability is typically linked with changes in hydrological and weather conditions (e.g. discharge, air temperature and rainfall), and among others (e.g. changes in vegetation cover/land use and land management practice) (Guo et al., 2018; Guo et al., 2019b; Hrachowitz et al., 2016; Jordan et al., 1997; Mosley, 2015; Scanlon et al., 2007; Schilling et al., 2017). Similarly, riverine water quality can vary markedly between catchments. The relationship between water quality and land use has been extensively studied and identified as one of the key controlling factors that affect spatial variation in water quality (Aronson et al., 2014; Bramley & Roth, 2002; Calijuri et al., 2015;

Hunter & Walton, 2008; Jiang et al., 2015; Lintern et al., 2018a; Nash & Chaloud, 2011). For instance, land clearing and any associated intensification of agricultural activities post clearing can result in an increase in nutrient loads from fertiliser application, as well as suspended sediment caused by altering surface soil properties (e.g., tillage) and sediment budgets (Blevins et al., 2018; Muscutt et al., 1993; Skaggs et al., 1994; Stonestrom et al., 2009). In addition, the natural conditions of catchments (e.g., climate, hydrology, geology and topography) have a potential impact on the spatial variation in water quality (Dillon & Kirchner, 1975; Donohue et al., 2006; Lintern et al., 2018b; Singh et al., 2004; Ye et al., 2009).

In this study, we focus on the spatial aspect of the water quality responses, acknowledging that temporal dynamics are also important (Guo et al., 2019b). Previous studies have highlighted a range of modelling techniques that can be used to explore the relationship between catchment characteristics and water quality responses (Afed Ullah et al., 2018; Ekholm et al., 2000; Fu et al., 2019; Letcher et al., 2002; Lintern et al., 2018b; Mainali et al., 2019; Singh et al., 2007; Soranno et al., 1996). However, these studies have certain limitations. Previous studies have mainly focused on a small number of catchment characteristics, mostly hydroclimatic and land uses characteristics (Afed Ullah et al., 2018; Jordan et al., 1997; Young et al., 1996). Also, despite efforts to monitor water quality in catchments worldwide, understanding of water quality spatial variation is still lacking for tropical and subtropical zones (Liu et al., 2018; Piazza et al., 2018). The mean or median of the long-term ambient water quality record might be inaccurate, due to the common practice of regular grab sampling with low frequency (e.g. often monthly) (Minaudo et al., 2017). More importantly, past investigations have often identified a 'best model' using forward or backward stepwise variable selection to interpret the complex processes (Juahir et al., 2011; Sangani et al., 2015; Singh et al., 2004). However, a single best model can be hard to confidently identify as multiple controlling factors can result in multiple plausible models that have similar predictive power (Whittingham et al., 2006).

This study aimed to: (1) identify the influential catchment characteristics affecting the spatial variability in different water quality constituents; and (2) develop a robust statistical modelling approach to predict the average water quality responses, using the key catchment characteristics in the tropical catchments. We used a long-term water quality event-based monitoring dataset of nine water quality constituents (i.e. sediment, nutrients and salinity), collected from 32 catchments in the Great Barrier Reef catchments (Queensland, Australia). We included 58 catchment-scale natural and anthropogenic characteristics in six categories: catchment topography, land cover, land use, geology, climate and hydrology, which were investigated to assess their relative effects on water quality spatial responses.

5.3 Materials and Methods

5.3.1 Study area

The Great Barrier Reef (GBR) is an iconic Australian coral reef ecosystem, with substantial environmental and economic value (De Valck & Rolfe, 2018; Whitten & Bennett, 2004). However, it has experienced a drastic decline in coral cover – 50% for the entire GBR – since 1985 (Brodie et al., 2013a; Kroon et al., 2016). This deterioration is thought to be driven in part by poor riverine water quality discharging from the adjacent catchments (Waterhouse et al., 2017). More detailed information on the location of 32 catchments can be found in Sections 3.3 and 4.3.1.

5.3.2 Data collection and preparation

5.3.2.1 Water quality data collection

Same water quality monitoring data was used, as described in Sections 3.3.2 and 4.3.2.

5.3.2.2 Runoff event delineation and event-mean concentration calculation

Individual runoff events were delineated based on the continuous discharge record extracted from the Water Monitoring Information Portal (DNRME, 2018). To identify the individual runoff event, we used an automated hydrograph analysis tool

– HydRun (Tang & Carey, 2017). The start and end points of a specific event were determined by using a local-minimum method through calculating the first derivative of streamflow (separated from baseflow). The event-mean concentration (EMC) was then calculated for each event that had at least two samples on both the rising limb and falling limbs of the hydrograph. This ensured sufficient samples taken over the runoff hydrograph, and the reliability of derived EMC (Waters & Packett, 2007). For each event, the EMC of a constituent was calculated as the total load per unit flow volume within the event (Joo et al., 2012), as follows:

$$EMC = \frac{Event\ Load}{Event\ Flow\ Volume} = \frac{\sum_{j=0}^{n} \frac{c_j + c_{j+1}}{2} \times q_{j+1/2} \times t_{j+1/2}}{\sum_{j=0}^{n} q_{j+1/2} \times t_{j+1/2}} \qquad \text{Equation 5-1}$$

where n is the total number of samples for a given event, c_j is concentration of the j^{th} sample, $q_{j+1/2}$ and $t_{j+1/2}$ are the inter-sample mean discharge and time interval between j^{th} and $(j+1)^{th}$ samples, respectively. We identified the concentration at the start and end of all events (c_0 and c_{n+1}) by assuming they were the average concentration of all baseflow samples. The EMCs we developed were essentially a flow-weighted mean concentrations over different runoff events, which allowed us to compare water quality across catchments with contrasting flow regimes (Cooke et al., 2000; Richards & Baker, 1993).

The site-level average of constituent EMCs (i.e., average of all available EMCs for each constituent at each site) were calculated (summary statistics are available in Table S-11) for use in statistical analysis. Prior to analysis, the site-level average EMCs for each constituent were Box-Cox transformed using car package in R (Fox et al., 2012), to improve the data symmetry (Box & Cox, 1964). For each constituent, the Box-Cox parameter λ was estimated individually. All the transformed variables were normally distributed based on the Shapiro-Wilk's test (see Appendix A2, Table S-12) (Shapiro & Wilk, 1965; Steinman et al., 2018).

5.3.2.3 Catchment characteristics data collection

Catchment boundaries of 32 sites were delineated using the Geofabric tool provided by the Australian Bureau of Meteorology (Bureau of Meteorology, 2012). We obtained the 58 different catchment characteristics (topography, land cover, land use, geology, climate and hydrology) from publicly available data sets (a brief summary in Table 5-1, and more details are in Table S-13 and Table S-14). Based on previous studies (Chang, 2008; Kleinman et al., 2004; Lintern et al., 2018a; Lintern et al., 2018b), these catchment characteristics were selected as they were potentially important factors driving the spatial variation in stream water quality. ArcGIS 10.5 was used to extract the catchment average from gridded raster (e.g. catchment rainfall) data or proportion of catchment coverage for polygon (e.g., land use) data. The 58 catchment characteristics were also transformed to better fit the linear model structure as detailed in Section 5.3.3. Log-sinh transformation was used here to handle zeros in the raw data (e.g., land use and hydrology characteristics) (Wang et al., 2012b). The transformation parameters for each catchment characteristic were obtained using the GA package in R (R Core Team, 2013; Scrucca, 2013). We also used the Shapiro-Wilk's test to evaluate the improvement in the normality of the transformed catchment characteristics (Table S-15). Some catchment characteristics were strongly cross-correlated (correlation matrix – Spearman's rank correlation coefficient in Figure S-8). Prior to the analyses, both response variables (i.e., EMCs in Section 5.3.2.2) and explanatory variables (i.e. 58 catchment characteristics) were standardized to a mean of 0 and standard deviation of 1 to enable comparison between explanatory variable regression coefficients (i.e., relative importance of model predictors) (Cade, 2015).

Table 5-1. Summary of selected catchment characteristics and data source (detailed summary in Appendix A2, Table S-13 and Table S-14)

Catchment characteristics	Min	Percentiles					Max	Source
		10th	25th	50th	75th	90th		
Topography								
Mean catchment elevation (m)	74	185	270	340	466	608	813	Geoscience Australia (2011)
Catchment area (km^2)	240	409	835	6999	17806	35188	139163	
Land cover								
Forest cover (%)	0.0	1.3	9.3	16.5	41.4	73.3	88.6	Geoscience Australia (2011)
Shrubs (%)	0.0	0.0	0.0	0.3	1.0	4.6	6.4	
Land use								
Grazing (%)	1.2	8.7	39.0	61.2	79.8	88.6	96.1	Queensland Government (2017b)
Sugar cane (%)	0.0	0.0	0.0	0.3	6.7	12.9	47.0	
Geology								
Catchment underlain by unconsolidated materials (e.g. colluvium and alluvial) (%)	0.0	1.5	7.3	21.9	32.8	52.1	76.9	Geoscience Australia (2011)
Mean TN levels in soil in catchment (mg/kg)	0.1	0.1	0.1	0.1	0.3	0.30	0.3	Terrestrial Ecosystem Research Network (2016)
Climate								
Average temperature (°C)	19	19	20	21	22	22	24	Geoscience Australia (2011)
Annual average rainfall (mm)	543	622	689	1139	1535	2719	3745	
Hydrology								
Average annual runoff (mm)	18557	96480	183384	461105	1081221	2717981	7045249	DNRME (2018)

5.3.3 Statistical analyses

We first mapped the time-averaged EMC values for the nine constituents across the GBR catchments. In addition, the correlation analysis between each pair of water quality constituents aimed to evaluate whether common patterns exist for different constituents. To assess the effect of each catchment characteristic, we used multi-model inference to investigate the key controlling catchment characteristics. Once the key catchment characteristics driving spatial differences in riverine water quality were identified, predictive models were built. Multi-model inference is a statistical technique that considers evidence from multiple plausible models, instead of a single 'best' model. Such a multi-model inference approach has been shown to be more robust than the conventional single-model approach, and less affected uncertainties in model selection (Burnham & Anderson, 2002; Poeter & Anderson, 2005; Saft et al., 2016). Multi-model inference in this study involves three steps, namely, (1) identification of multiple plausible models using linear regression, (2) predictions using a model-averaging technique and (3) model assessment. The analyses were performed in MATLAB version R2017b (MATLAB and Statistics Toolbox, 2017).

5.3.3.1 Identification of plausible models

To identify the plausible models to predict average EMCs for each constituent, and reduce the computational burden, we adopted a two-round Exhaustive Search approach (i.e. two stages in Figure 5-1) (Guyon & Elisseeff, 2003; Lintern et al., 2018b; May et al., 2011; Saft et al., 2016). We used ordinary least square to fit the all candidate models in both rounds of an exhaustive search.

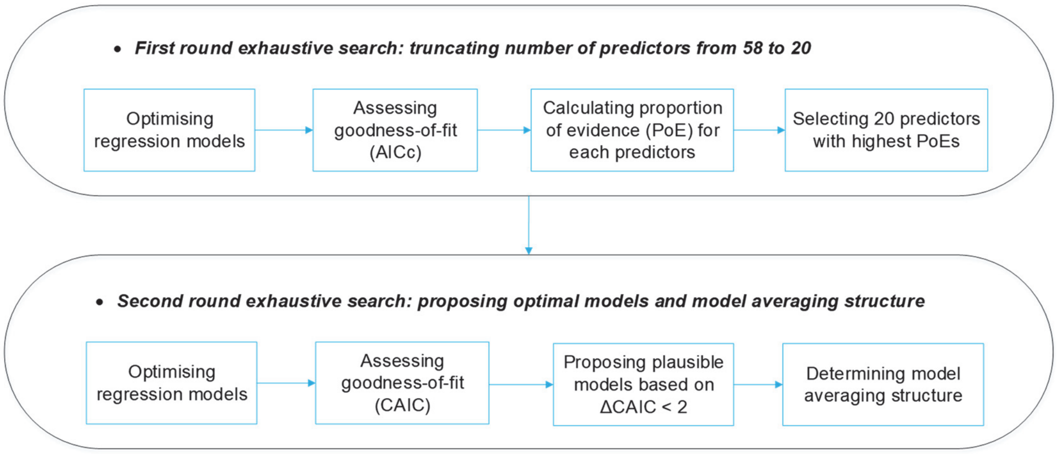

Figure 5-1. Analysis stages in identification of plausible models.

In the first round of the Exhaustive Search, we aimed to truncate the number of predictors to a more manageable level. Then, all possible combinations of predictors - up to a maximum of five predictors - were used to construct linear additive models to predict EMCs (Lintern et al., 2018b; Saft et al., 2016). To account for the randomness and uncertainties in observations, for each constituent the model fitting was performed 20 times, each with 26 sites that were randomly selected (approximately 80% of the total number of sites). This resulted in 91,642,320 models (20 repetitions × 4,582,116 models for each replicate) to be compared for each constituent in this round.

We assessed and compared all possible models derived from the first round using the Corrected Akaike Information Criterion (AICc), which is preferred for small sample applications (Hurvich & Tsai, 1989). The model weights w_i is calculated as follows,

$$w_i = e^{-0.5\Delta AIC_{Ci}} / \sum_{n=1}^{N} e^{-0.5\Delta AIC_{Cn}} \qquad \text{Equation 5-2}$$

where N is total number of models, and ΔAICc is the difference in AICc between model i and the minimum AICc.

Model weights were used to estimate the relative importance of individual explanatory variables by summing w_i for each model in which that explanatory variable appears. This is defined as the Proportion of Evidence (PoE) for each predictor (Mohan et al., 2018; Saft et al., 2016). If a predictor appears more frequently in models with small Δ_i (i.e. higher relative performance), then the PoE of that predictor is close to 1. This allowed us to consider the relative importance of individual exploratory variables across all models, and hence identify key predictors. We calculated the average PoE for each catchment characteristic and retained the 20 catchment characteristics with the highest PoE for the second round of the exhaustive search.

This smaller number of predictors allowed us to explore more possible combinations of explanatory variables while reducing computational requirement. Thus, we fitted all possible models with up to 10 predictors for each constituent. The final model retained for model averaging were all those that included predictors with the minimum subjects per variable (SPV, ratio of number of observations to number of predictors) larger than 3. This should result in adequate estimates of regression coefficients (Austin & Steyerberg, 2015).

5.3.3.2 Model averaging

We used a different information criterion, i.e. Complete Akaike Information Criterion (CAIC) to assess each model (Bozdogan, 1987) and identify the model averaging structure to predict average water quality conditions. The reason we used CAIC is because it penalizes complex models more heavily. We identified plausible models as models with a CAIC difference ($\Delta CAIC_i$) less than 2 (Burnham & Anderson, 2002).

The predictions of the individual plausible models were averaged using the weighting coefficients defined by ΔCAIC, similar to the method we used to calculate the model weights w_i (Equation 5-2, but calculated based on ΔCAIC). The model weights were then used to compute model-averaged predictions, defined as:

$$\overline{\boldsymbol{y}} = \sum_{i=1}^{N} w_i \boldsymbol{y_i} \qquad \text{Equation 5-3}$$

where $\mathbf{y_i}$ is a vector of the estimated EMCs across all sites, w_i is the weighting coefficients for model i, N is total number of plausible models ($\Delta CAIC_i < 2$) for each constituent and $\overline{\boldsymbol{y}}$ is a vector of the weighted predictions.

To compare the effects of predictors selected in the plausible models on the response variable, the averaged parameter coefficients ($\overline{\beta}_j$, Equation 5-4) and corresponding variance ($var(\overline{\beta}_j)$, Equation 5-5) can be calculated as follows,

$$\overline{\beta}_j = \sum_{i=1}^{N} w_i \beta_{i,j} \qquad \text{Equation 5-4}$$

$$var(\overline{\beta}_j) = \sum_{i=1}^{N} w_i [var(\beta_{i,j}) + (\beta_{i,j} - \overline{\beta}_j)^2] \qquad \text{Equation 5-5}$$

where $\beta_{i,j}$ and $var(\beta_{i,j})$ are the fitted model coefficients and corresponding variance of predictor j in a given model i, and w_i is the weight of model i. $\overline{\beta}_j$ and $var(\overline{\beta}_j)$ were only averaged over the models that included the predictor of interest (i.e. $\beta_{i,j}$ = 0 if predictor j was not included in model i) (Lukacs et al., 2010).

5.3.3.3 Model assessment

The averaged model predictions were evaluated using the Nash-Sutcliffe coefficient (NSE) (Nash & Sutcliffe, 1970). A residual assessment was performed to check: (1) normality of the residual, (2) heteroscedasticity in residuals (i.e. no clear relationship between residual and predictors that were included in the model averaging structure), and (3) the residuals were randomly and independently distributed across space. For (3), Moran's I was calculated using model residuals and the inverse Euclidean distance approach (Chen, 2013; Mainali & Chang, 2018; Mainali et al., 2019; Miralha & Kim, 2018). Generally, Moran's I ranges from -1 to 1, indicating dispersion and clustering, respectively. The significance of the spatial autocorrelation was tested based on the p-value of Moran's I (note that the null hypothesis is that residuals are randomly distributed across space).

Two additional assessments were performed. Firstly, to compare the relative importance of the natural and anthropogenic (i.e., land use) catchment characteristics, the averaged model structure was re-calculated using only natural catchment characteristics (i.e. land use characteristics were excluded). Secondly, to assess the robustness of the averaged model and quantify the uncertainty in predictions, we conducted a five-fold cross validation. The entire set of catchments (32) was randomly divided into 80% (26) and 20% (6) subsets, with the 80% subset of the data used for calibrating the averaged models. The predictive performance of the calibrated model was validated against the excluded 20% of the catchments. This was repeated 5,000 times to obtain an ensemble of predictions for each site and to eliminate the effect of sampling. This reduced potential bias resulting from the difference in the number of calibration and validation sites. The NSE of calibration sites was calculated by randomly taking 6 sites out of 26 calibration sites, so that the number of calibration and validation sites in the NSE calculation was the same. By comparing the two distributions of NSEs from 5,000 cross-validation runs, we assessed the robustness of the model structure.

5.4 Results

5.4.1 Spatial pattern of averaged EMCs

The average EMC of the nine constituents showed different spatial patterns across the GBR catchments (Figure 5-2). Generally, the particulate constituents, i.e., TSS, PN and PP, exhibited a similar pattern, where averaged EMCs were lower in the northern region and increased towards the southern sites (Spearman's Rank cross-correlations among these three constituents $\rho > 0.76$, $p < 0.01$, Figure 5-3). A similar pattern was observed for the dissolved species (e.g. NH_4, DON, FRP, relationships $\rho > 0.45$, $p < 0.01$, Figure 5-3); however, averaged NO_X showed a contrasting spatial pattern, with sites in the coastal regions (e.g., the Wet Tropics and Mackay-Whitsunday) having much higher averaged EMCs compared with other sites.

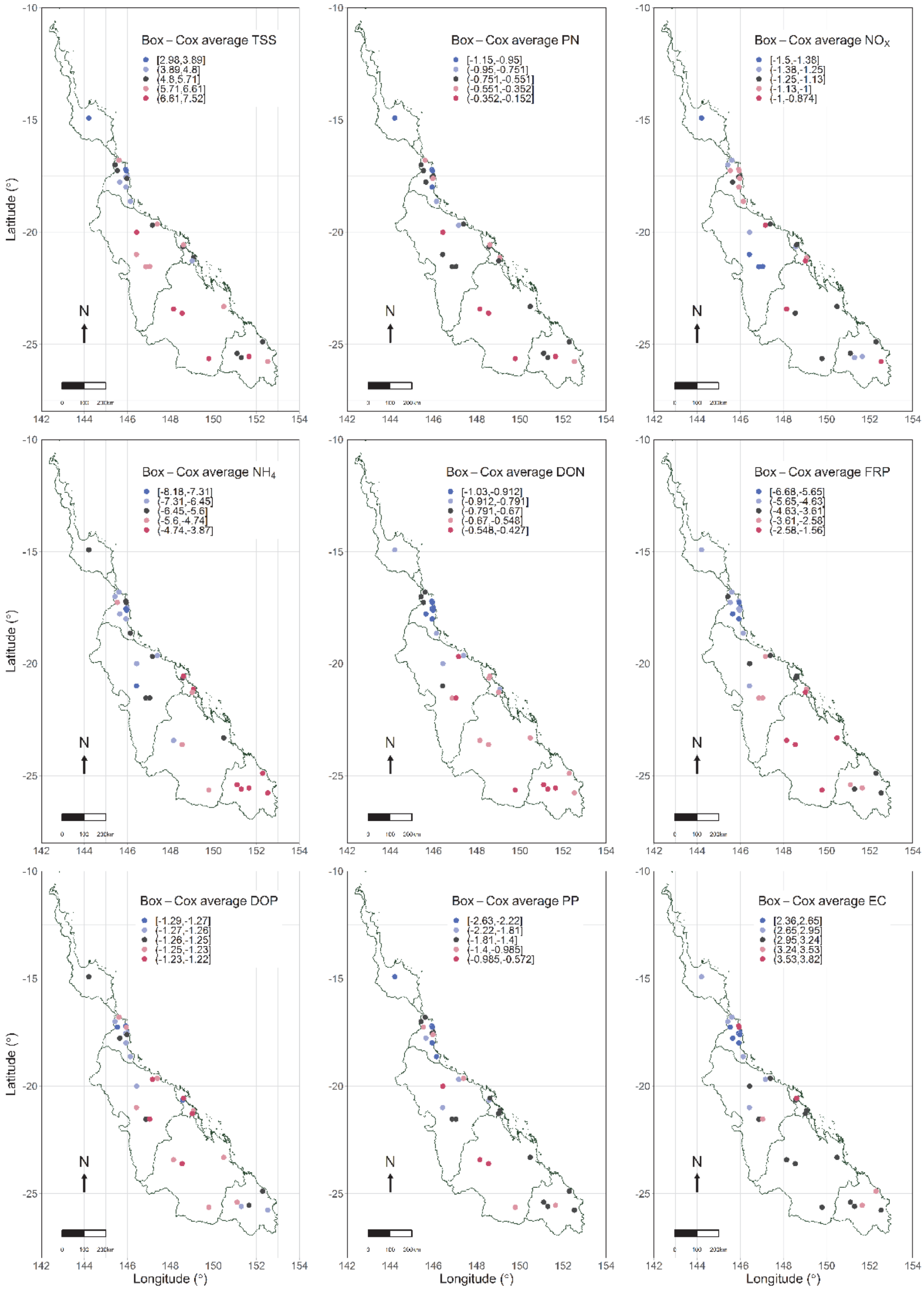

Figure 5-2. Averaged EMC of nine constituents across the 32 GBR catchments. Colour indicates relative magnitude, blue – low and red – high.

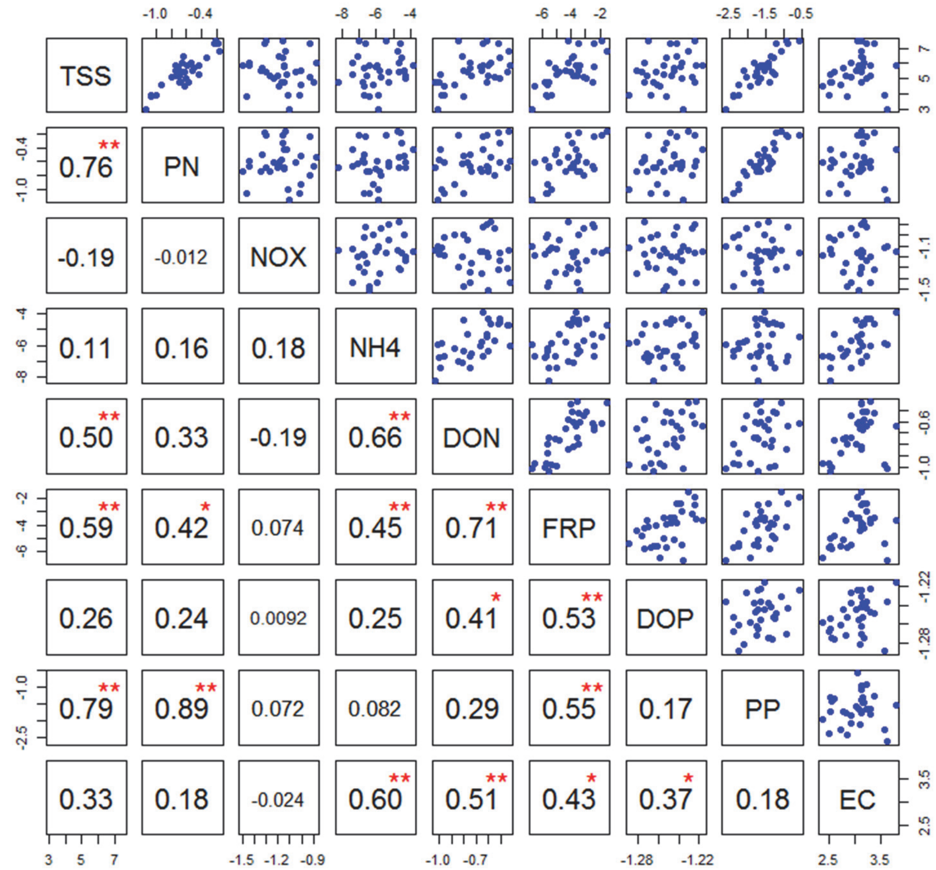

Figure 5-3. Spearman Rank correlations among averaged transformed EMCs of nine constituents (** and * indicate significance at $p < 0.01$ and $p < 0.05$, respectively).

5.4.2 Multimodel inference on modelling of spatial variability in EMCs

5.4.2.1 Key factors identified in plausible models

The effect of each catchment characteristic on average EMCs varied between different constituents (PoEs in Figure 5-4, Figure S-9 and Figure S-10). Results from here on will focus mainly on three constituents (i.e., TSS, NO_X and FRP), due to their relatively high risk to the receiving marine environment, where all other six constituents are in Section A2 in Appendix. Catchment geological and climatic characteristics were more likely to be included in the plausible models for the particulate constituents (i.e., TSS, PN and PP). Additionally, the results showed that there was a stronger relationship between catchment land cover and land use types and dissolved inorganic nitrogen (i.e., NO_X and NH_4), compared with other constituents. For DON, DOP and EC, there were consistently higher numbers of important catchment characteristics from multiple categories. It was also worth noting that catchment hydrology was only identified as an important factor for DON and NO_X.

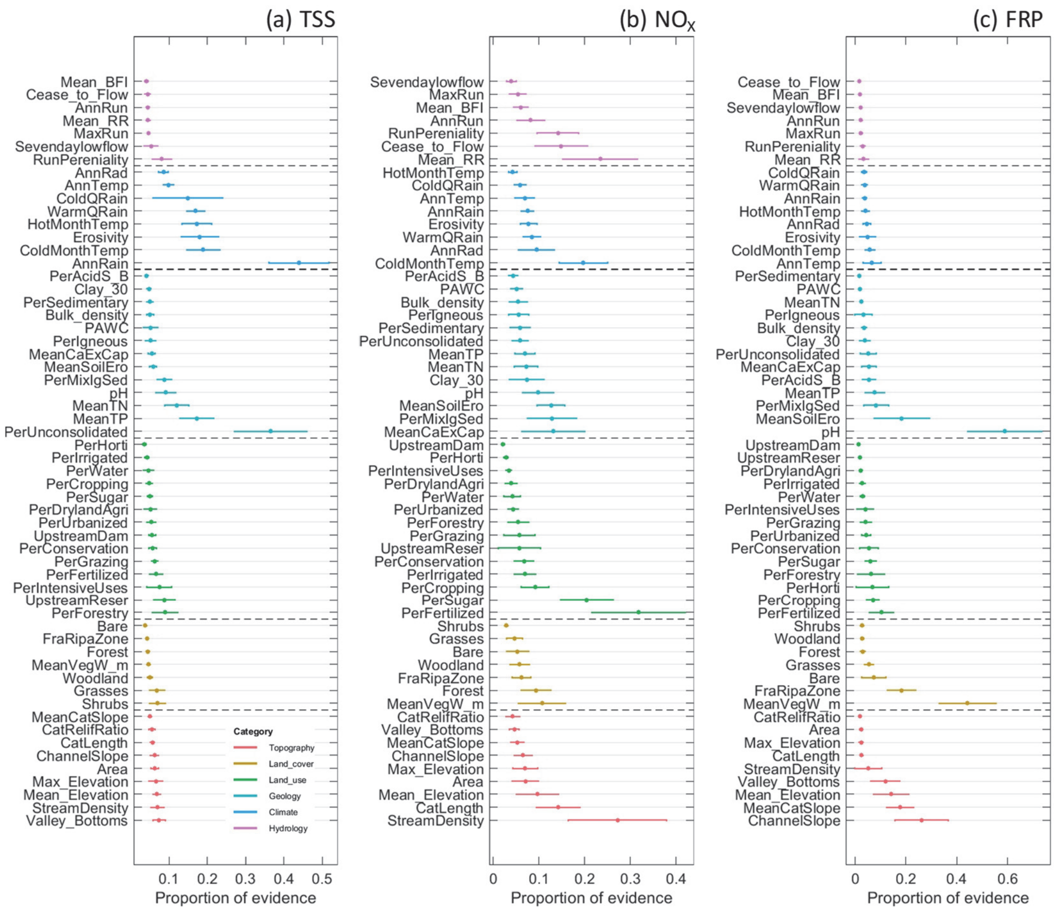

Figure 5-4. Proportion of Evidence (PoE) of each catchment characteristics for: (a) TSS; (b) NO_X and (c) FRP. Dot represents the average of PoE from 20 subsampling tests, with horizontal bar indicates the ± one standard deviation. Catchment characteristics within each category (represented by six different colours, see legend in panel a) were plotted in a descending order of the corresponding average PoE. The definition of abbreviation of each catchment characteristic can be found in Appendix A2, Table S-13.

5.4.2.2 Model-averaging performance

The number of plausible models determined from the second round of the exhaustive search for each constituent ranged from 2 for FRP to 26 for PP (a detailed summary of each likely model is available in Table S-16). NSE ranged from 0.64 for PN to 0.98 for DON (Table 5-2). The weighted parameter coefficients and proportion of evidence of selected catchment characteristics in the final plausible models varied across different constituents (TSS, NO_X and FRP in Figure 5-5, for the other constituents see Figure S-11 and Figure S-12). In addition, the exclusion of anthropogenic characteristics resulted in a large decrease in NSE for DOP (-31%), NO_X (-30%) and NH_4 (-14%) (Table 5-2) but had a minimal effect on the other constituents. The residual analysis showed no clear heteroscedasticities in model residuals (from Figure S-13 to Figure S-20), and residuals were normally distributed by a visual check (Figure S-21) and the Shapiro-Wilk's tests (all p-value > 0.01, Table 5-2). Most constituents had negative Moran' I in residuals (Table 5-2), indicating weak dispersion of model residuals. However, significant spatial dependency was only found in residuals of NH_4 and DOP models.

Table 5-2. Model averaging performance and weighted predictor coefficients. NSE and Moran' I in residual were calculated based on averaged predictions across all identified plausible models. The third and fourth columns are averaged model performance when considering only natural catchment characteristics (i.e., land use landscape factors are excluded), and the change in NSE compared to full model, respectively.

Constituent	NSE full model	NSE - only natural catchment characteristics included	% change in NSE	Number of plausible models	Moran' I in residual	Shapiro-Wilk's test p-value in residuals
TSS	0.75	0.75	0%	14	-0.08	0.97
PN	0.64	0.62	-3%	8	-0.11	0.38
NO_X	0.83	0.58	-30%	3	-0.18	0.47
NH_4	0.89	0.76	-14%	15	-0.23*	0.85
DON	0.98	0.98	0%	15	-0.16	0.45
FRP	0.95	0.88	-8%	2	-0.01	0.02
DOP	0.71	0.49	-31%	10	-0.26**	0.33
PP	0.79	0.79	0%	26	-0.17	0.99
EC	0.87	0.79	-9%	10	0.02	0.06

Note: **and * indicate spatial autocorrelation is significant at $p < 0.01$ and $p < 0.05$, respectively. Shapiro-Wilk's test p-value > 0.01 indicates the acceptance of the null hypothesis that data comes from a normal distribution at the 1% significant level.

The cross-validation results demonstrated a good fit between the median of predictions and observations, regardless of calibration or validation sites (see Figure S-22 to Figure S-24). This is further evidenced by the comparison between the distribution of the calibration and validation NSEs for each of the 5,000 runs, in which the validation runs showed a slight decrease in the median NSE (Figure S-25).

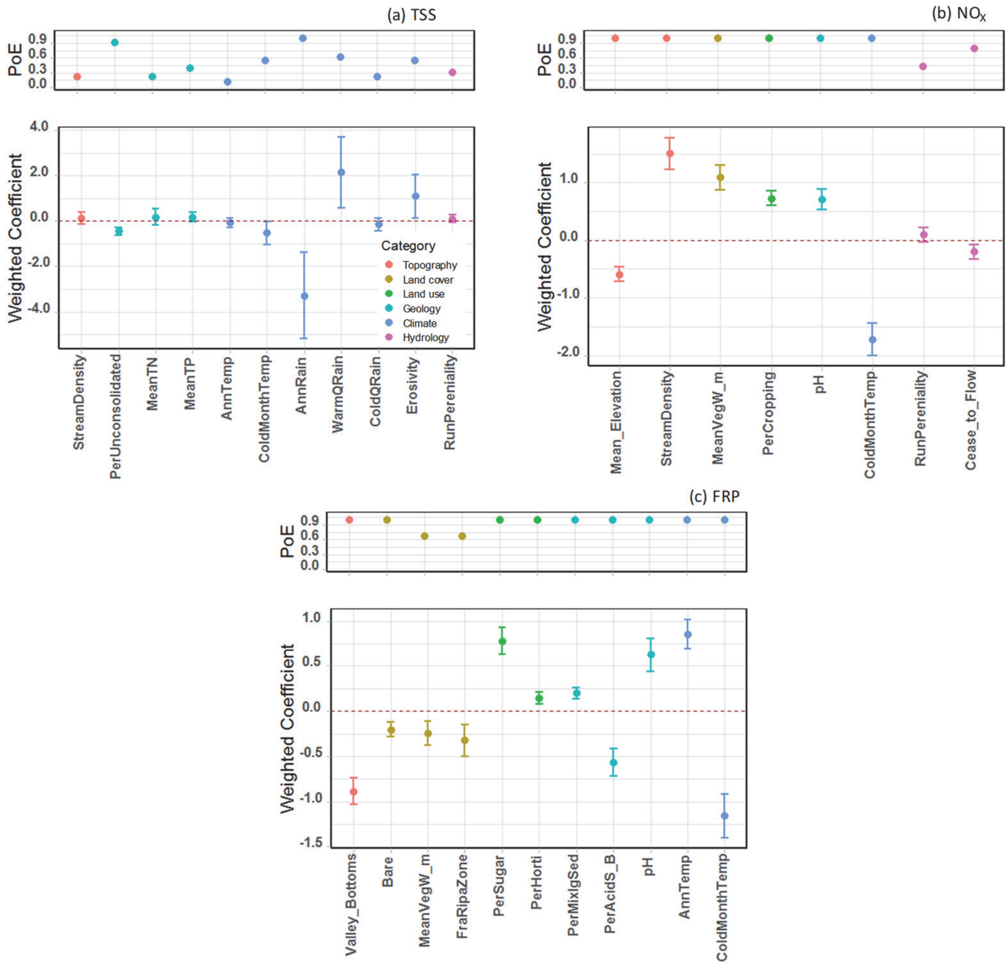

Figure 5-5. Weighted coefficients and Proportion of Evidence (PoE) of catchment characteristics selected in the final plausible models for: (a) TSS; (b) NO_X and (c) FRP. Bottom panel indicated the mean (dot, $\bar{\beta}_j$, Equation 5-4) and standard deviation (error bar, $\sqrt{var(\bar{\beta}_j)}$, Equation 5-5) of the weighted coefficient for each selected catchment characteristics, and different color represents each category (see legend in panel [a]). The definition of abbreviation of each catchment characteristic can be found in Table S-13.

5.5 Discussion

5.5.1 Influential factors affecting spatial variation in stream water quality

5.5.1.1 Statistical inference for the relative importance of natural and anthropogenic landscape characteristics

Catchment natural characteristics were more important than anthropogenic landscape factors. Exclusion of anthropogenic predictors in model building did not influence the prediction performance of TSS, PN, PP and DON markedly (Table 5-2). This indicates that spatial differences in averaged EMCs of these constituents (especially for particulate species) are better explained by natural characteristics of catchments in the statistical models. In addition, a relatively small performance drop for FRP and EC suggested that land use measures were secondary explanatory variables and have limited effects on the results. In contrast, land use measures (e.g. proportion of sugar) had high predictive power for DOP, NO_X and NH_4, demonstrating that in the GBR catchments specific land use was an important driving factor in spatial variability of EMCs of dissolved constituents across catchments. These results are consistent with previous findings that land use changes are related to sources of dissolved forms of nutrients in the GBR catchments (Brodie et al., 2003; Hunter & Walton, 2008; O'reagain et al., 2005). In general, catchment natural characteristics exhibited higher predictive capability than catchment anthropogenic characteristics. Indeed, natural catchment characteristics might have a direct impact on human-induced landscape factors, e.g. agricultural activities are strongly influenced by climate conditions (Hatfield et al., 2011; Thorburn et al., 2013). As a result, spatial variation in water quality is better predicted by catchment natural landscape characteristics. This might be also a reflection of the nature of the data-driven approach to variable selection, that means we could potentially omit a factor that is related to key water quality processes if it is correlated with another non-causal factor. Thus, when catchment natural characteristics were included, the multi-model structure tended to avoid including catchment anthropogenic characteristics.

5.5.1.2 Climate

Climatic variables had high PoEs and consequently were included in the plausible models for all constituents (Figure 5-4, Figure S-9 and Figure S-10). Air temperature was identified as a key factor among these climatic characteristics. It is not surprising since temperature affects almost all physio-chemical processes and biological reactions for nutrients (Huang et al., 2003; Lintern et al., 2018a; Sardans et al., 2008; Tockner et al., 1999). The average lowest minimum temperature in each year (ColdMonthTemp) had a strong negative effect on NO_X, NH_4, DON and FRP, indicating higher nutrient levels were generally associated with catchments experiencing colder winter months. In our study region, climate has a clear seasonal distinction that features high flow events in the wet/hot summer (typical time when the EMCs are derived), but rarely in the relatively cold/dry winter. During the cold/dry periods, nutrients stored in soil are more likely to be stabilized and accumulated in the soil, such that there are increases in nutrient availability for the subsequent summer wet season (Edwards & Withers, 2008; Houser & Richardson, 2010; Pionke et al., 1999; Young et al., 1996). In contrast, the average highest maximum temperature (HotMonthTemp) had a positive effect on PP and PN. This could be attributed to an increased rate of mineralization and release of nutrients (in particulate form) with higher temperature (Zhu et al., 2005; Zwolsman & Van Bokhoven, 2007), and higher erosion rate due to increased pollutant transport capacity (higher rainfall and runoff) during the hot wet season (Delpla et al., 2009).

Annual rainfall (AnnRain) was another controlling factor with a consistently negative impact on TSS, PN, DON, and EC. This result contrasts with previous studies in other catchments (Cavelier et al., 1997; Granger et al., 2010; Perona et al., 1999). The contrast between our results and the existing understanding of the impact of rainfall might be due to the high interaction between rainfall and land use/land cover in the GBR catchments. For example, an inverse relationship between annual rainfall and grazing land use ($\rho = -0.89$, $p < 0.01$, Figure S-8) shows that grazing agriculture is mostly conducted in dry catchments (e.g. the Fitzroy and Burdekin regions). These catchments contribute a large proportion of sediments to the GBR, due to a higher potential for gully and hillslope erosion (Kuhnert et al., 2012; McKergow et al., 2005b; Waterhouse et al., 2017).

5.5.1.3 Topography

Catchment topographic characteristics were identified as important factors for dissolved nutrients and salinity. Catchment elevation was included in the final plausible models for NO_X, NH_4, DON and EC, with negative weighted regression coefficients. Meanwhile, there is a positive effect of catchment slope on NH_4 and EC. These factors are relevant to pollutant mobilisation and delivery. In GBR catchments, low-elevation, small coastal catchments are relatively steeper with a high relief ratio (Figure S-8). For pollutants strongly influenced by subsurface runoff transport processes (e.g. NO_X, NH_4 and EC), concentrations tend to increase with slope but decrease with elevation (Clow & Sueker, 2000; Skoulikidis et al., 2006; Young et al., 1996). Prasad et al. (2005) found the similar results that NH_4 and NO_X concentrations during events were correlated positively with catchment slope and negatively with elevation. These topographic features also influence aquifer dynamics that control the fraction of groundwater in surface runoff (Skoulikidis et al., 2006). Lower-lying land is typically associated with higher groundwater contribution, leading to an increase in the concentration of dissolved nutrients and salts in streams (Kratz et al., 1997; McKergow et al., 2003).

The large effects of stream density for NO_X and NH_4 (Figure 5-4[b] and Figure S-11[b]) could potentially be explained by the catchment export processes for inorganic nitrogen, which are strongly controlled by density of stream network (Alexander et al., 2002a; Prasad et al., 2005). There are two possible reasons for the difference in direction of impact (positive for NO_X and negative for NH_4). Firstly, catchments with denser stream networks are more likely to have shorter runoff pathways to receiving waters. This leads to more rapid delivery of NO_X with less losses from denitrification (Young et al., 1996). Secondly, the negative feedback between ammonia nitrogen and stream density might be due to the cross-correlation between stream density and land cover (Figure S-8). Biogeochemical processes in forest and riparian vegetation (e.g. assimilated by phytoplankton) would reduce the dissolved inorganic nutrient levels (Tabacchi et al., 2000). Compared to NO_X, this effect has a more direct impact on NH_4 as it is more prone to plant uptake (Bernhardt et al., 2002; Bronk et al., 1994).

5.5.1.4 Geology

Catchment geological and soil were important for all constituents, except for NH_4. Catchment lithology was one of the most frequently selected predictors. The percentage of catchment underlain by regolith – unconsolidated materials (e.g. colluvium and alluvial deposits) (PerUnconsolidated) has a negatively weighted regression coefficient for particulate species, i.e. TSS, PN and PP. However, the positive regression coefficients of mixed sedimentary and igneous rock (PerMixIgSed) for FRP, DOP and PP demonstrate that sedimentary and igneous deposits may act as a source of these constituents. Phosphate minerals can be derived from sedimentary and igneous deposits (mainly in forms of phosphorites and apatite, respectively), and the release of dissolved phosphorus in phosphate is enhanced due to weathering and hydrological transport (Holtan et al., 1988; Pufahl & Groat, 2017). During the wet season in the GBR catchments, the increased water availability is likely to enhance the erosion and chemical weathering processes of the bedrocks (Bouchard & Jolicoeur, 2000). The weathered material tends to be transported via surface and subsurface runoff, leading to an increase in levels of both sediment-bound and dissolved phosphorus (Hattanji & Onda, 2004; Pelletier & Baker, 2011). There is negative feedback between this process and the thickness of regolith (e.g. unconsolidated materials), such that catchments underlain by deeper unconsolidated materials might experience lower levels of particulate and dissolved nutrient species (Strudley et al., 2006).

Soil characteristics (e.g. pH) had high PoE for several constituents. Soil pH has a positive effect on FPR and NO_X in their respective model averaging structures. This can be explained by the fact that the soil acidity affects biogeochemical processes. Specifically, dissolved phosphorus fixation by irons is enhance by lower soil pH (Hinsinger, 2001; White, 1981). Lower soil pH also prevents the denitrification process of oxidized nitrogen due to the poor adaptation of denitrifying microbials to acidic environments (Simek & Cooper, 2002).

5.5.1.5 Land cover

The impact of natural land cover characteristics in the GBR catchment were not as evident as geological and topographic characteristics. It was only identified as an important predictor for dissolved nutrients (e.g. NO_X, DON, DOP and FRP).

We note that the mean width of vegetated riparian zone along streams (MeanVegW_m) had a contrasting influence on NO_X (positive) and FRP (negative). Generally, nutrients are inversely correlated with riparian vegetation cover due to their reduction via biogeochemical processes (e.g. plant uptake and denitrification) and sedimentation of particulate forms (Chang, 2008; Johnson et al., 1997; Varanka et al., 2015). However, our results indicate that the effect of riparian vegetation on oxidized nitrogen is the opposite to such expectations. In the GBR catchments, a large proportion of NO_X export occurs in the Wet Tropics, where large amounts of fertiliser is applied on sugarcane crops (Rayment, 2003; Thorburn et al., 2013). NO_X is more prone to leach through soil via travel in subsurface hydrological pathways. Our results on the effect of riparian vegetation is supported by findings from McKergow et al. (2003) and Meynendonckx et al. (2006), who found elevated levels of NO_X as a result of a shorter residence time and greater contribution from subsurface flow pathways in wet catchments. However, it is also worth noting that the positive effect of riparian vegetation on sediment and nutrient removal has been identified in many studies in the GBR catchments (Arnaiz et al., 2011; McKergow et al., 2004) and elsewhere in the world (Osborne & Kovacic, 1993; Wang et al., 2011; Wilcock et al., 2009). Another possible explanation was the data source of riparian vegetation. The riparian vegetation information used in the study was measured using Landsat satellite imagery, and a buffer of 100m on both sides of rivers and riverine wetlands was considered to assess the riparian area (Clark et al., 2015; Queensland Government, 2016). This might introduce certain bias when the actual width of riparian zone is less than the spatial resolution of the Landsat imagery (i.e., 30 meters) (Woodcock et al., 1994). Therefore, to obtain a more nuanced understanding of the effects of specific land cover on spatial differences in water quality using statistical analyses, further investigation is required with continuous water quality monitoring data and finer-scale vegetation surveys (e.g. from both remotely-sensed products and in-situ measurements) (Goodrich et al., 2000; Johansen & Phinn, 2006).

5.5.1.6 Land use

Agricultural activity (e.g. sugar and horticulture) had a positive relationship with NO_X, NH_4, FRP, DOP and EC, indicating these anthropogenic controlled land uses might act as sources of instream pollutants. This accords with previous studies that concluded sediment, nutrients and salts in rivers are likely to be sourced from agricultural activities (Afed Ullah et al., 2018; Allan et al., 1997a; Little et al., 2005; Liu et al., 2018; Teixeira et al., 2014; Yan et al., 2013).

The effect of land use is particularly evident for dissolved inorganic nitrogen (i.e. NO_X and NH_4) and dissolved phosphorus (i.e. DOP, FRP). Results suggest that sugarcane (PerSugar) and cropping (PerCropping) are two prominent factors. It is worth noting that these two predictors were collected from two different sources (see Appendix A2, Table S-13), and percentage of cropping included sugarcane. Therefore, they somehow overlapped. There is a clear association between inorganic nitrogen and sugarcane production in the GBR catchments, with the majority of the GBR sugarcane concentrated in the Wet Tropics and Mackay-Whitsunday (Bainbridge et al., 2009b; Hunter & Walton, 2008). Higher inorganic nitrogen (Figure 5-2) might be linked with fertiliser application and losses through surface and subsurface pathways (Little et al., 2005; Liu et al., 2017b). While percentage of catchment fertilized (PerFertilized) and sugar were two contributory factors identified in the first round of Exhaustive Search (Figure 5-3), they were not included in the multimodel structure for NO_X. This can be explained by the high cross-correlation between these factors and cropping activity (Figure S-8), with cropping alone explaining the spatial differences in NO_X.

5.5.1.7 Hydrology

Catchment hydrological characteristics showed high PoEs only for dissolved nitrogen species (i.e. NO_X, NH_4 and DON) and salinity. Runoff perennially (percentage contribution to mean annual discharge by the six driest months of the year) appears as a predictor with strong explanatory power for DON and NH_4. The result is not surprising since catchment hydrology is highly correlated with other catchment characteristics (e.g., $\rho = -0.85$ for runoff ratio and grazing agriculture, and $\rho = 0.82$ for baseflow index and soil TN level, Figure S-8). Prathumratana et al. (2008) found that the inter-correlation between catchment runoff, temperature and rainfall could explain the spatial variation of sediments and nutrients in the lower Mekong River. A possible reason is that catchment hydrology is more likely to affect the temporal variation in water quality rather than spatial variability (Chen et al., 2007). However, the negative effect of the runoff perennially on DON and NH_4 implies that EMCs of dissolved nitrogen are strongly affected by the proportion of wet season runoff volume contributing to the annual runoff (e.g. Joo et al. (2012)).

5.5.2 Predicting spatial variation in averaged EMCs

The statistical modelling framework proposed in this study was pragmatic and provided a simple approach for assessing average water quality conditions during runoff events across a large tropical region. The weighted prediction derived from the model averaging approach performed relatively well and captured a large proportion of spatial variability in water quality. Within all constituents we studied, we had better ability to predict the dissolved nutrient species than particulate pollutants. This is in contrast to our earlier study (i.e. Lintern et al. (2018b)), where we investigated the linkage between spatial variability in average water quality and catchment characteristics in 102 catchments in Victoria, Australia. The contrasting results can be explained by difference in water quality data. Firstly, the water quality monitoring data in our study focused on runoff events, rather than the monthly sampling used in Lintern et al. (2018b). We considered the variability in streamflow when developing EMCs using event-based water quality samples, thus reducing the uncertainty associated with concentrations of monthly samples. This might result in that the averaged EMCs of dissolved nutrients were more strongly influenced by catchments' natural characteristics (e.g. hydrology for NO_X and geology for FRP). Secondly, these two studies also have the following specific differences in key processes driving dissolved and particulate pollutants: 1) land use (e.g. sugarcane) has a clear linkage to dissolved nutrients in our study area but there is no sugar cane and less intensive cropping in the Victorian catchments, and 2) the two study areas have contrasting climates (tropical and temperate), leading to, among other differences, flow regimes and rainfall being more variable in the GBR catchments compared to Victoria. In addition, it is worth noting that the significant spatial autocorrelation in model residuals of NH_4 and DOP (Table 5-2) might be related to other catchment landscape factors (e.g. land management practice) that are not included in this study. This leads to geographical distance among different catchments became an influential factor that affect the unexplained variation in these constituents (Mainali & Chang, 2018; Mainali et al., 2019).

Our modelling was developed with multi-model inference. Compared to the conventional single best model approach (Ekholm et al., 2000; Sangani et al., 2015; Varanka et al., 2015), multi-model inference greatly extended our ability to address uncertainties arising from model (variable) selection and associated dependence between coefficient values and variables included by considering multiple plausible models (Cade, 2015; Parrish et al., 2012; Ye et al., 2008). These uncertainties are quantified by the model weights or probabilities (Akaike weights, Table S-16) and incorporated into the interpretation of weighted model predictions and regression coefficients of key catchment characteristics. A comparison of the distribution of NSEs from our five-fold cross validation results (Figure S-25) demonstrate the robustness of the model averaging approach. This suggests that applying this statistical approach to other regions with water quality issues would be useful.

5.5.3 Management implications and future research

Catchment pollutant management requires us to recognize the importance of a wide range of catchment characteristics, especially how the effects of changes (e.g. in land use, land management, land cover or climatic condition under climate change) alter pollutant export during runoff events. Our analyses show that catchment anthropogenic characteristics are more pertinent to dissolved nutrients (e.g. NO_X, NH_4). Therefore, continuous monitoring of changes in land use and management, as well as the water quality responses in these intensively used catchments would provide improved insight into managing nutrient sources. This is in line with the current improved management practice adopted in the GBR catchments (Star et al., 2018; Thorburn et al., 2013). Our results also indicate that spatial variability in particulate pollutants are more directly influenced by a catchment's natural characteristics. This does not necessarily imply that the land use is unimportant for particulate constituents. For example, grazing is the dominant land use in the GBR catchments. Hence, departures from this land use (e.g. presence of sugarcane) may be more useful in predicting water quality spatial variation than the amount of grazing per se. Therefore, grazing still needs to be considered when determining management strategies for sediment and particulate nutrients, e.g. control of gully and streambank erosion (Bartley et al., 2014b; Bartley et al., 2007; Thorburn & Wilkinson, 2013). Future analysis of temporal variation in water quality is required to assess dynamics of the sediment and particulate constituents. Investigation of the factors such as catchment vegetation canopy cover, which is influenced by grazing, will test this hypothesis.

A limitation of this study is that the investigation focused solely on the averaged water quality conditions for runoff events. While this might be useful for the long-term planning of improved management practice, it does not provide insight into the temporal variation in water quality responses. Future analyses will investigate the driving factors (e.g. changes in discharge and land cover) that influence the temporal variability in water quality, which is also of great importance (Brodie et al., 2010; Guo et al., 2019b). The incorporation of spatial and temporal modelling frameworks would provide comprehensive understanding of how water quality changes across space and over time. In addition to this, it is noted that pesticides, posing a direct threat to the GBR lagoon ecosystems (Haynes et al., 2000; Lewis et al., 2009), were not included in this study. Further investigation could extend our existing modelling framework to include these emerging chemicals.

5.6 Conclusions

In this study, a data-driven statistical approach was used to identify the important factors affecting the spatial differences in water quality in the Great Barrier Reef catchments. Our results indicate the catchment natural characteristics have higher explanatory power in this statistical modelling framework. They are more influential on spatial water quality variations than human-induced factors, although land use is strongly related to dissolved nutrient concentrations. The models developed were able to predict average event-mean concentrations well (NSE ranging from 0.64 to 0.98). The proposed multi-model framework, therefore, could be used to identify potential hotspots of water quality concerns, at unmonitored locations. This modelling framework also enables valuation of water quality responses to future changes in climate or land use. With ongoing water quality monitoring data available at multiple GBR catchments, further investigations focusing on temporal variability in water quality are essential to advance our understanding of water quality dynamics.

Chapter 6 Key Factors Influencing Temporal Variability in Stream Water Quality in the Great Barrier Reef Catchments

This chapter is currently under internal review and will be submitted to the journal, Water Resources Research as the following article:

Liu, S., Ryu, D., Webb, J., Lintern, A., Waters, D., Guo, D., & Western, A. (2019). Key factors influencing temporal variability in stream water quality in the Great Barrier Reef catchments. Water Resources Research, under internal review.

6.1 Abstract

Stream water quality is highly variable both in space and time. Water quality monitoring programs have collected a large amount of data that provide a good basis to investigate the key drivers of spatial and temporal variability. Event-based water quality monitoring data in the Great Barrier Reef catchments in northern Australia provides an opportunity to further understand water quality dynamics in sub-tropical and tropical regions. This study investigated nine common water quality constituents, including sediments, nutrients and salinity, with the aim of: 1) identifying the influential environmental drivers of temporal variation in flow event concentrations; 2) comparing these across catchments and constituents; and 3) predicting the temporal variation in water quality at multiple sites simultaneously. This study used a hierarchical Bayesian model averaging framework to explore the relationship between event concentration and catchment-scale environmental variables (e.g., runoff, rainfall and groundcover conditions). Key factors affecting the temporal changes in water quality varied among constituents, as well as between catchments. Catchment runoff and rainfall affected particulate constituents, while catchment wetness and vegetation cover had more impact on dissolved nutrients and salinity. In addition, in large and dry catchments, antecedent catchment soil moisture and vegetation had a greater influence on dissolved nutrients, indicating the effect of catchment hydrological connectivity on pollutant mobilisation and delivery.

The key points of this chapter are:

- A Bayesian hierarchical modelling approach coupled with Bayesian model averaging is used to assess the impacts of hydroclimatic and vegetation cover conditions on temporal variation in water quality.
- The identified key hydroclimatic and vegetation cover conditions vary among different constituents, and across different catchments.
- The established models perform better for dissolved nutrients, possibly due to controls of catchment hydrological connectivity on dissolved nutrients mobilisation and delivery.

6.2 Introduction

In-stream water quality plays a vital role in influencing the health of freshwater ecosystems (Bhaduri et al., 2016; Pérez-Gutiérrez et al., 2017), which in turn determines environmental, social and economic sustainability (Hanjra & Qureshi, 2010; Kontogianni et al., 2003; McGrane, 2016). Non-point source pollution derived from agricultural land and urban development have led to water quality degradation in streams and lakes in many regions of the world (Novotny, 1999; Peters & Meybeck, 2000; Ren et al., 2003; Sharpley, 2016). Among these water quality issues, coastal regions with high agricultural production have been delivering large amounts of pollutants to the ocean, where marine ecosystems are vulnerable to the evaluated levels of nutrients and sediments (Carpenter et al., 1998; Gorman et al., 2009). It is estimated that 60% of coastal rivers in the USA have been moderately to severely degraded (Gorman et al., 2009; Howarth et al., 2002). Therefore, to protect both freshwater and marine ecosystems, better management of catchment-derived pollutants is needed.

Surface water quality is highly variable in space and time (Allan et al., 1997a; Guo et al., 2019b; Lintern et al., 2018a). These spatial and temporal variations are the result of complex interactions between three key pollutant processes in catchments, namely, sources (e.g., atmospheric deposition or anthropogenic inputs), mobilisation (e.g. detachment from the sources), and delivery (e.g. transport from sources to receiving waters) (Granger et al., 2010; Lintern et al., 2018a). Across different catchments, spatial differences in water quality concentration can vary markedly due, in part, to heterogeneity of natural landscapes in a catchment (e.g. geology, topography and climate) and human-induced activities (e.g., agricultural and urban development) (Liu et al., 2018; Mainali & Chang, 2018; Mainali et al., 2019). At a site, water quality concentration can also exhibit significant daily, event, seasonal and annual variability, driven by variations in climatic conditions, in-stream biogeochemical processes and hydrological transport (Hill, 1996; Pretty et al., 2006; Thompson et al., 2011). Thus, it can be challenging to design effective catchment water quality management strategies without a sound understanding of the spatial and temporal variation in water quality and the associated driving factors.

While it has been acknowledged that both spatial and temporal variations in water quality are of great importance for effective water resources management (Guo et al., 2019a), this study focused on identifying key drivers of the temporal variability in water quality. It follows our previous study investigating spatial variation in water quality in the same region (Liu et al., 2018). A wide range of environmental factors may affect temporal changes in water quality. Runoff and rainfall have been considered as important factors and the most commonly used explanatory variables to describe temporal variation in water quality (Deletic & Maksimovic, 1998; Kim et al., 2007; Yang et al., 2009), for example early work by Hem (1948), Walling and Foster (1975) and Walling (1984). Studies considering hydrometeorological drivers have been typically related to the mobilisation and delivery of pollutants. Catchment soil moisture and evapotranspiration can also have an important role in determining the hydrological cycle (e.g., runoff generation), such as sediments (Bieger et al., 2014; Varanou et al., 2002), nutrients (Bouraoui et al., 2002; Lam et al., 2010) and salinity (Brevik et al., 2006; Tweed et al., 2007), thereby affecting the surface water quality. In addition, riverine water quality can be strongly influenced by seasonal changes in vegetation cover (de Mello et al., 2018; Griffith et al., 2002; Shi et al., 2017). For instance, satellite-derived vegetation indices have provided an opportunity to explore the relationship between land cover and water quality temporal dynamics (Fu & Burgher, 2015; Griffith, 2002; Singh et al., 2013; Whistler, 1996). Even though significant research efforts have been made to explore the relationship between water quality and these environmental conditions, a comprehensive understanding their relative importance in diverse environments and at large scales is still lacking.

Statistical modelling has been widely used to investigate water quality temporal dynamics in response to changes in the abovementioned environmental factors (Alexander et al., 2002b; Fu et al., 2019; Kroon et al., 2016; Kuhnert et al., 2012; Miller et al., 2014; Singh et al., 2013; Zhang & Blomquist, 2018; Zhang et al., 2016a; Zhang & Schilling, 2005). For example, a flexible generalized additive modelling (GAM) framework has been used to characterise flow and concentration relationships for estimating loads at GBR catchments (Kroon et al., 2012; Kuhnert et al., 2012). However, existing studies have limitations. First, the water quality monitoring data have often been limited to low sampling frequencies, typically using monthly grab samples. This may have resulted in a lack of information on water quality dynamics over runoff/storm events, when a significant proportion of nutrients and sediment loads are transported (Lloyd et al., 2016; Sherriff et al., 2015). Second, most water quality modelling studies have only investigated the relationship between water quality and explanatory variables in a single or limited number of catchments in small regions (Liu et al., 2008b; Zhang et al., 2016a). Few studies have investigated water quality at multiple locations using the same modelling framework. Lastly, studies have usually relied on a single 'best' model with an assumption that it best approximated the true drivers of water quality (Paliwal et al., 2007; Zhang et al., 2009b). Ignoring the issue of selection uncertainty and relying on a single model structure might result in misleading conclusions or overconfidence in the results. This model-selection uncertainty, as well as the question of which predictors can be credibly included in a predictive water quality model have rarely been acknowledged (Link & Barker, 2006; Wintle et al., 2003).

This study attempted to address the above deficiencies using event-based water quality monitoring data from the Great Barrier Reef (GBR) catchments in northern Australia, where land-derived pollutants have posed threats to ecosystems of the GBR lagoon (Brodie et al., 2012; Hunter & Walton, 2008; McKergow et al., 2005b; Waterhouse et al., 2017). We targeted nine common water quality indicators, involving sediments, nutrients and salinity. Bayesian hierarchical modelling was used to investigate water quality temporal variation. This allowed the prediction of water quality in multiple catchments, as well as simultaneously quantify parameter uncertainty. In addition, we used Bayesian model averaging (BMA) approaches to identify the relative importance of the different environmental factors and provide multi-model weighted predictions, which have been shown to better quantify the uncertainty arising from model selection (Höge et al., 2019; Raftery et al., 1997; Wang et al., 2012a). This study aimed to: (1) identify the key drivers of temporal variation in water quality; (2) compare these drivers across catchments and constituents; and (3) predict water quality temporal variation using a Bayesian multi-model approach.

6.3 Materials and Methods

6.3.1 Study area

Description of the study area can be found in Sections 3.3 and 4.3.1. Thirty-two sites within the GBR catchments were selected as case study catchments. Previous multivariate analysis of the spatial patterns of time-averaged concentrations indicated that, there were two groups of sites (Figure 4-3), which was a result of spatial heterogeneity in catchment landscape characteristics (Liu et al., 2018).

Table 6-1. Summary of differences in landscape characteristics between the two clusters of sites (Liu et al., 2018).

Cluster	Climate	Hydrology	Land use/land cover	Topography
1	Wet tropics region with high annual rainfall	Perennial, high energy rivers	Dominated by conservation (e.g. rainforest), and cropping (e.g. sugar)	Small and steep
2	Mostly dry tropics, relatively dry with clear seasonal variability in rainfall	Ephemeral, low energy rivers, cease-to-flow in dry period	Dominated by brigalow native vegetation, and pastures for grazing,	Large and flat

6.3.2 Data collection and preparation

6.3.2.1 Water quality data

Same water quality monitoring data was used, as described in Sections 3.3.2 and 4.3.2.

6.3.2.2 Event mean concentration

We extracted continuous discharge records for each site from the Water Monitoring Information Portal (DNRME, 2018) to identify individual runoff events. The detailed method of the EMCs calculation can be found in Section 5.3.2.

The EMCs were essentially flow-weighted mean concentrations over individual runoff events, which allowed the comparison of water quality across catchments with contrasting flow regimes (e.g., two clusters of sites in Figure 4-3) (Cooke et al., 2000; Richards & Baker, 1993). A total of 1412 events was identified across the 32 sites, and, depending on data availability, EMCs were calculated for between 21% (DOP) and 43% (TSS) of these identified runoff events (see Appendix A3, Table S-17).

The derived EMCs were Box-Cox transformed to improve the symmetry of the response variable (Box & Cox, 1964) to improve model fitting (Hawkins & Weisberg, 2017; Lawrance, 1988; Zhang & Yang, 2017). The site-level Box-Cox transformation parameter λ for each constituent was first identified, using the car package in R (Fox et al., 2012; R Core Team, 2013). Then, for each constituent, the average λ from the 32 sites was used to transform all available EMCs for that specific constituent. This ensured that an identical transformation parameter was applied across the different sites for each constituent (Guo et al., 2019b).

6.3.2.3 Time-varying catchment characteristics

This study investigated the effect of various hydrologic, climatic and vegetation cover characteristics for different events. These characteristics involved runoff, catchment root zone soil moisture, actual evapotranspiration rainfall, air temperature, and vegetation cover. The continuous streamflow monitoring data, gridded weather and climatic products, and remotely-sensed imagery were used to derive catchment average conditions for each event (see Table 6-2).

Table 6-2. Time-varying catchment characteristics and their data sources.

<table>
<tr><th>Explanatory variable</th><th>Unit</th><th>Spatial resolution</th><th>Source</th></tr>
<tr><td>Daily runoff</td><td>mm/d</td><td>point measurements</td><td>Queensland Department of Natural Resources, Mines and Energy (DNRME, 2018). Available from https://water-monitoring.information.qld.gov.au/</td></tr>
<tr><td>Daily rainfall</td><td>mm</td><td rowspan="2">5 km × 5 km</td><td rowspan="2">Australia Water Availability Project (AWAP) (Raupach et al., 2009). Available from http://www.csiro.au/awap/</td></tr>
<tr><td>Daily temperature</td><td>°C</td></tr>
</table>

16-day NDVI	-	1 km × 1 km	Moderate Resolution Imaging Spectroradiometer (MODIS) - MOD13A2v006 (Didan, 2015). Available from https://earthdata.nasa.gov/
Daily soil moisture (root zone 0 -100 cm)	mm	5 km × 5 km	Australia Landscape Water Balance model (AWRA-L) (Frost et al., 2016). Available from http://www.bom.gov.au/water/landscape
Daily actual ET	mm		

Note: ET – evapotranspiration

For individual runoff events identified in the previous section, three groups of event characteristics were prepared, characterising pre-event, during-event and post-event conditions (Table 6-3). Except for runoff, data for all explanatory variables were first extracted from gridded data using catchment boundaries were delineated using the Geofabric tool provided by the Australian Bureau of Meteorology (Bureau of Meteorology, 2012). The catchment average time series data were then averaged over the specific time-window related to the event (see Table 6-3).

Table 6-3. Three groups of event characteristics and averaging method.

Group	**Explanatory variable**	**Abbreviation used in figures and tables**	**Calculation method**
During-event	Average runoff	Event_ave_Q	Average of daily runoff during event
	Maximum runoff	Event_max_Q	Maximum of daily runoff during event
	Average rainfall	Event_ave_P	Average of daily rainfall during event
	Maximum rainfall	Event_max_P	Maximum of daily rainfall during event
	Average temperature	Event_T	Average of daily temperature during event
	Average NDVI	Event_NDVI	Average of NDVI during event
	Average soil moisture	Event_SM	Average of daily soil moisture during event
	Average actual ET	Event_AET	Average of daily actual ET during event
Pre-event	Average runoff	Ante_Q	Average of daily runoff for 7 days prior to event
	Average rainfall	Ante_P	Average of daily rainfall for 7 days prior to event
	Average NDVI	Ante_NDVI	Average of NDVI for 3 months prior to event

	Average soil moisture	Ante_SM	Average of daily soil moisture for 7 days prior to event
	Average actual ET	Ante_AET	Average of actual ET for 7 days prior to event
Post-event	average runoff	Post_Q	Average of daily runoff for 7 days after event

Note: Q – runoff; P – rainfall; T – temperature; NDVI – normalized difference vegetation index; SM – root zone soil moisture; ET = evapotranspiration.

The explanatory variables in the during-event conditions were averaged over the duration of the event. For the pre-event and post-event conditions, the 7 days prior to and after the event were used as the time-window (except NDVI). The 7-day period was the median of the time of concentration (i.e., the time for runoff to travel from the most remote point of the catchment to the monitoring site) across all catchments. These were estimated from catchment topography using the Bransby-William's equation, following its wide application in Australian catchments for flood estimation (French et al., 1974; Pilgrim et al., 1987). The ground cover was quantified by NDVI, an indicator of the biophysical condition of the vegetation canopy (Griffith et al., 2002). Previous studies have also shown that there is a time-lag between water availability and a change in ground cover, which is typically three months for Australian catchments (De Keersmaecker et al., 2015; Papagiannopoulou et al., 2017). Therefore, to represent the pre-event ground cover condition, we averaged all available NDVI measurements for three months prior to an event. The runoff after the event (7 days) was also included as an indicator of catchment wetness at the end of the event, to assess if hydrologic condition towards the end of an event influences the temporal variation in water quality.

Similar to the EMCs, all the explanatory variables were Box-Cox transformed, following the procedure described in Section 6.3.2. In addition, prior to the analyses, both transformed EMCs and explanatory variables were standardized to a mean of zero and standard deviation of one. As such, the magnitude of a coefficient indicates the effect of each predictor relative to other predictors (Wan et al., 2014b). The cross-correlation (non-parametric Spearman's Rank correlation coefficient) of all transformed predictors is provided in Appendix A3, Figure S-25.

6.3.3 Modelling: driver identification and water quality prediction using multi-model inference

Several steps were involving in the statistical analyses (Figure 6-1). The overarching modelling structure is linear model that predicts temporal variation in water quality, as well as incorporates a combination of catchment drivers (e.g. hydroclimatic conditions). This enables the comparison of relative importance of different divers on temporal variation in water quality. In addition, Bayesian approach was used to incorporate the inherent stochasticity in water quality into the modelling framework. The Bayesian modelling framework was applied to site Clusters 1 ('wet') and 2 ('dry') separately (derived from cluster analysis in Chapter 4), to identify the difference between key drivers of temporal variability in water quality and to assess the predictive performance.

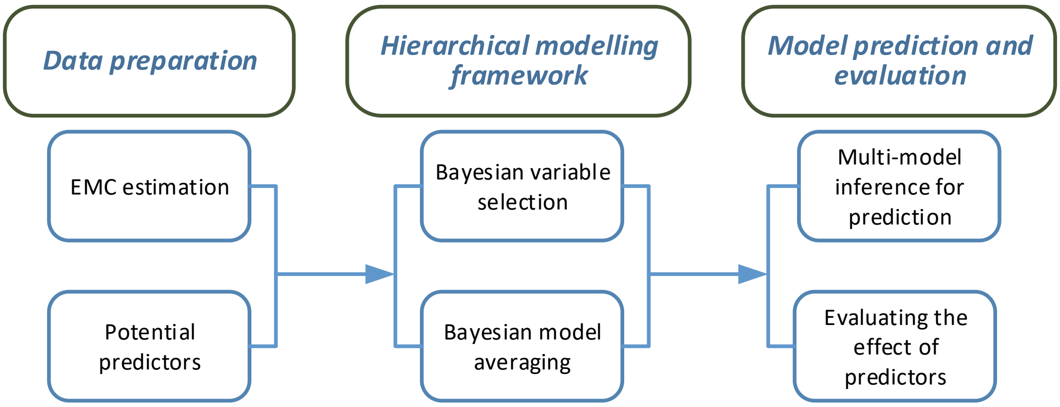

Figure 6-1. Analyses steps; the detailed methods used in the hierarchical modelling framework and model prediction and evaluation are in the following sections.

6.3.3.1 Bayesian variable selection

To investigate the relative importance of individual predictors, an indicator Bayesian variable selection method was used, called Gibbs variable selection (GVS) (George & McCulloch, 1993; Ntzoufras, 2002). An auxiliary inclusion variable I_n (Equation 6-1) for each predictor was introduced to indicate whether that predictor was 'in' or 'out' of an individual iteration of the hierarchical modelling structure.

$$I_n = \begin{cases} 1, \text{ n}^{\text{th}} \text{ predictor present} \\ 0, \text{ n}^{\text{th}} \text{ predictor absent} \end{cases} \quad \text{Equation 6-1}$$

I_n was modelled at the top level of the hierarchy which enabled use of identical model structures (i.e., a combination of predictors) across different sites. The overarching hierarchical modelling framework was defined as follows:

$$y_{i,j} \sim N(\mu_{i,j}, \sigma) \quad \text{Equation 6-2}$$

$$\mu_{i,j} = \overline{mean}_j + \overline{std}_j \times \Delta_{i,j} \quad \text{Equation 6-3}$$

$$\Delta_{i,j} = \sum_{n=1}^{N} \theta_{n,j} \times x_{n,i,j} \quad \text{Equation 6-4}$$

$$\theta_{n,j} = I_n \times \beta_{n,j} \quad \text{Equation 6-5}$$

The data-level model Equation 6-2) assumed that EMC of a particular constituent (e.g., one of TSS, NO_X, EC, etc) at i^{th} time step in the j^{th} sub-catchment, $y_{i,j}$, followed a normal distribution (denoted as N(·)), with mean $\mu_{i,j}$ and a global standard deviation σ. The mean value, $\mu_{i,j}$ was modelled as the observed site-level averaged EMC $\overline{mean}_j$ plus $\overline{std}_j \times \Delta_{i,j}$, with the latter term being defined as the deviation from this averaged value (Equation 6-3) (Guo et al., 2019b). The deviation term incorporated the site-level observed standard deviation $\overline{std}_j$, making $\Delta_{i,j}$ a standardised measure that could be compared across sites. $\Delta_{i,j}$ was further modelled as a linear additive function (Equation 6-4) of all candidate predictors x_n in n = 1, 2, …, N = 14 (e.g., event average runoff, rainfall and NDVI). Consequently, $\Delta_{i,j}$ was defined as temporal variability in water quality, and was the quantity of interest. The effect size ($\theta_{n,j}$) of individual predictors was another latent variable used in the GVS, and was estimated as the product of I_n and the regression coefficient $\beta_{n,j}$ (Equation 6-5), such that $\theta_{n,j}$ was either $\beta_{n,j}$ (I_n = 1), or 0 (I_n = 0).

6.3.3.2 Hierarchical prior specification and Bayesian inference of key drivers

Bayesian inference required the specification of the prior distributions for each model parameter. A minimally-informative uniform prior (denote as U(·)) between 0 and 10 was assigned to the global standard deviation (σ, Equation 6-6) (Gelman, 2006). The prior distribution of I_n assumed that each indicator came from an independent Bernoulli distribution, with a probability of 0.5 (Equation 6-7) (Raftery et al., 1997). This vague prior results in each model structure having an equal prior model probability.

$$\sigma \sim U(0,10) \qquad \text{Equation 6-6}$$

$$\mathrm{P}(I_n = 1) \sim Bernoulli(0.5) \qquad \text{Equation 6-7}$$

A hierarchical conditional prior specification for predictor coefficients was used, which allowed the site-specific parameter values that described the effects of each temporal predictors ($\beta_{1,j}$, $\beta_{2,j}$..., $\beta_{n,j}$) to be exchangeable between sites (Liu et al., 2008a; O'Hara & Sillanpää, 2009; Webb & King, 2009). The prior of $\beta_{n,j}$ was conditioned on I_n, resulting in a mixture distribution with 'slab and spike' prior, which was defined as follows:

$$\beta_{n,j} \left| I_n \sim I_n N(0,\tau_n) + (1-I_n) N(0,\tau_{n,tune}) \right. \qquad \text{Equation 6-8}$$

where $\beta_{n,j}$ | $(I_n = 1)$ is the slab part of the mixture distribution. The $\beta_{n,j}$ | $(I_n = 1)$ was estimated by including a higher-level distribution. The prior of $\beta_{n,j}$ | $(I_n = 1)$ followed a normal distribution with random effects (Equation 6-9), with the τ_n drawn from a common prior distribution, defined as a hyperparameter (i.e., uniform distribution between 0 to 20, Equation 6-10) (Gelman, 2006; Kruschke, 2014).

$$\beta_{n,j} \left| (I_n = 1) \sim N(0,\tau_n) \right. \qquad \text{Equation 6-9}$$

$$\tau_n \sim U(0,20) \qquad \text{Equation 6-10}$$

For the spike component, a data-dependent prior was specified for $\beta_{n,j}$ | $(I_n = 0)$, drawing from a pseudo-prior (Equation 6-11), that is, a prior distribution with no effect on the posterior distribution, but facilitating the mixing of the Gibbs sampler.

$$\beta_{n,j} \left| (I_n = 0) \sim N(0,\tau_{n,tune}) \right. \qquad \text{Equation 6-11}$$

This study estimated $\tau_{n,tune}$ from the standard deviations of the posterior of the $\beta_{n,j}$ in a global model structure (i.e., modelling structure using all predictors), as suggested by Carlin and Chib (1995) and Linden and Roloff (2015). The prior of

$\beta_{n,j} \mid (I_n = 0)$ was near the posterior estimates to facilitate mixing in the MCMC (Hooten & Hobbs, 2015).

The posterior inclusion probability (PIP - $P(I_n = 1|\boldsymbol{y})$, Equation 6-12) of each predictor was used to compare the relative importance of individual predictors (i.e., how often the n[th] predictor was 'in' the model).

$$P(I_n = 1|\boldsymbol{y}) = \frac{1}{T}\sum_{t=1}^{T} I(I_n^{(t)} = 1) \qquad \text{Equation 6-12}$$

where T is the total number of iterations of Markov chains. The different combination of I_n at each MCMC sampling represents a specific model structure. According to Bayes' theorem, the posterior model probability (PMP – $P(M_k|\mathbf{y})$) can be estimated as,

$$P(M_k|\boldsymbol{y}) = \frac{[\boldsymbol{y}|M_k]P(M_k)}{\sum_{x=1}^{L}[\boldsymbol{y}|M_x]P(M_x)} \qquad \text{Equation 6-13}$$

where L is the total number of possible models, and $P(M_k)$ is the prior probability of model M_k, among a group of models M_x, x = 1, …, X. This posterior model probability was obtained by assessing the frequency of a particular combination of I_n during the MCMC sampling.

6.3.3.3 Prediction from multi-model inference

We used Bayesian Model Averaging to generate an ensemble of predictions of temporal variation in EMC for individual constituents (Equation 6-14). The average posterior distribution of a quantity of interest (i.e., temporal variability in EMC) was generated using the parameters (e.g., $\beta_{1,j}$, $\beta_{2,j}$..., $\beta_{n,j}$) sampled from the posterior distribution to simulate EMC values using the specific model, defined as follows:

$$[\hat{\boldsymbol{y}}|\boldsymbol{y}] = \sum_{x=1}^{L}[\hat{\boldsymbol{y}}|\boldsymbol{y}, M_x]P(M_x|\boldsymbol{y}) \qquad \text{Equation 6-14}$$

where $[\hat{\boldsymbol{y}}|\boldsymbol{y}, M_x]$ is the posterior distribution of a vector $\hat{\boldsymbol{y}}$ of (prediction) derived from model M_x (Hooten & Hobbs, 2015; O'Hara & Sillanpää, 2009).

6.3.3.4 Model evaluation and implementation

The proposed modelling framework was applied to the two site clusters independently. This allowed an investigation of whether the spatial heterogeneity in catchment landscapes led to differences in the key factors controlling temporal variation in water quality. The key drivers were determined as the predictors with a PIP above 0.8 (i.e., over 80% of the models included these predictors).

To further understand the reliability and robustness of the BMA framework, the consistency of the posterior inclusion probability of individual predictors was investigated by resampling subsets of the observations multiple times (Kohavi, 1995). For each cluster, 80% of events within one site were first randomly selected and the posterior inclusion probability for this subset of observations was estimated. This was repeated 1,000 times to produce a distribution of posterior inclusion probabilities for individual predictors, which was then used to assess the uncertainty in the posterior inclusion probability.

An ensemble of the averaged prediction in temporal variability of each runoff event was obtained from each iteration of parameter updating using Markov chain Monte Carlo (MCMC). The model fit was evaluated using the Nash-Sutcliffe coefficient (NSE) (Nash & Sutcliffe, 1970) between the observed temporal variability and the median of ensemble predictions $\hat{\boldsymbol{y}}$ derived from the BMA (Equation 6-14). The NSE was calculated at both the cluster- and site-levels. The model residuals were also checked for normality and heteroscedasticity (i.e., relationship between the residual and predictors). In addition, model performance was evaluated by providing the 50% and 95% credible interval (CI) of each prediction.

To compare the relative importance of the predictors that have been widely used in existing literature (i.e., runoff and rainfall) and other predictors (e.g., soil moisture, temperature, evapotranspiration, and vegetation cover), the modelling framework was re-calibrated using only the rainfall/runoff related predictors (including all pre-, during- and post-event predictors). This estimated the degree of improvement in the model's explanatory power with the inclusion of environmental variables, such as catchment wetness and ground vegetation cover conditions.

The hierarchical modelling framework was implemented in JAGS (Plummer, 2003, 2013a), using the package rjags in R (Plummer, 2013b; R Core Team, 2013), which enabled both the estimation of parameter values from prior distributions with Markov chain Monte Carlo (MCMC) and the generation of model-averaged predictions. The MCMC sampling had three parallel chains with 25,000 iterations for each chain. The first 5,000 iterations were discarded as a 'burn-in' period to allow convergence of the Markov chains, resulting in 60,000 values to estimate the posterior distribution for each model parameter and make model predictions. The convergence of each chain was evaluated by plotting the trace plot and using the potential scale reduction factor; the Gelman-Rubin statistic ($\hat{R}$, $\hat{R} < 1.1$ when chains converged) (Gelman et al., 2013).

6.4 Results

6.4.1 Key drivers of temporal variability in water quality

The three key measures used in Clusters 1 and 2 presented in this section are: (1) estimates of posterior inclusion probability (PIP), which quantifies relative importance of individual predictors; (2) posterior model probability (PMP), which estimates differences in plausible model structures; and (3) posterior distributions of coefficients for the key drivers (effect size, e.g., $\theta_{1,j}$, $\theta_{2,j}$..., $\theta_{n,j}$ in Equation 6-4), which measures direction and magnitude of the effect of key predictors on water quality temporal variability.

Posterior inclusion probability (Figure 6-2 and Appendix A3, Table S-18) from the Bayesian modelling results indicated that, in general, antecedent vegetation condition and antecedent soil moisture were key factors in explaining temporal variation in water quality, especially for Cluster 2 (warmer and drier) sites. Catchment runoff and rainfall were the second most important group of factors, especially for particulate pollutants (TSS, PN and PP; Clusters 1 and 2) and salinity. In addition, the three groups of predictors (pre-, during-, post-event) had varying effects across different constituents. With regard to during-event conditions, event average runoff (Event_ave_Q), event maximum runoff (Event_max_Q) and event average rainfall (Event_ave_P) were three important factors with relatively high PIP. In contrast, among pre-event conditions, antecedent NDVI (Ante_NDVI) and antecedent soil moisture (Ante_SM) were driving factors for the majority of the constituents. Post-event runoff (Post_Q) only affected a few constituents (e.g., on NO_X and FRP for Cluster 2 and EC), compared with the other two groups of predictors. Overall, there were notable differences in the important predictors for Clusters 1 and 2, and many more important predictors were found for the Cluster 2 sites.

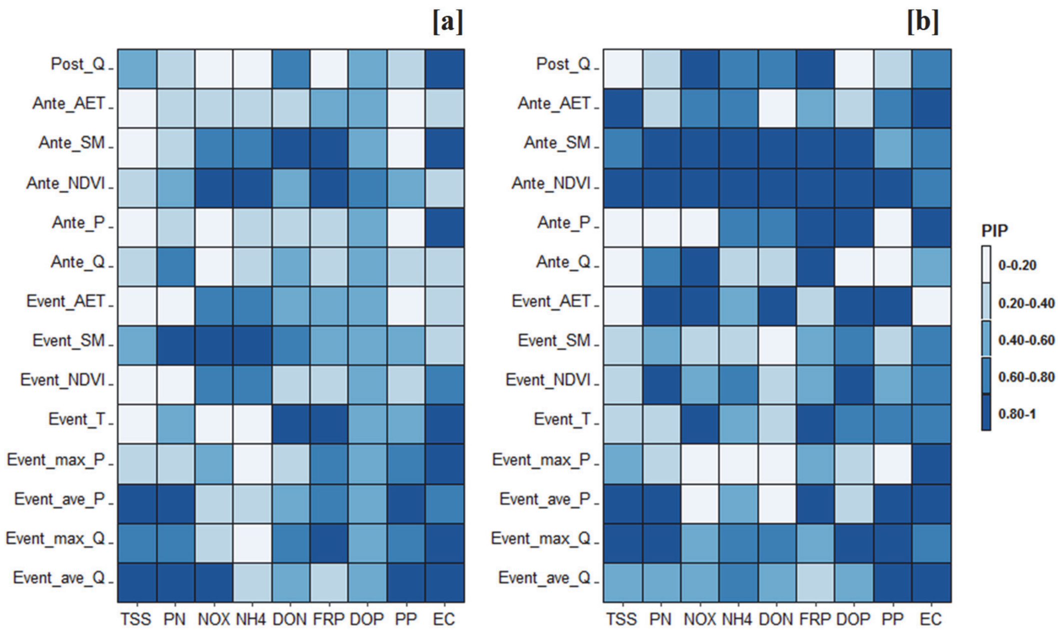

Figure 6-2. Posterior inclusion probability (PIP) of each candidate predictor for [a] Cluster 1 (“wet”) catchments, and [b] Cluster 2 (“dry”) catchments; dark blue = high PIP; light blue = low PIP. The definition of the abbreviations of each predictor on the y-axis are in Table 6-3.

Results from here on will focus mainly on three constituents (i.e., TSS, NO_X and FRP), due to their impacts on the marine receiving environment. Results for the other six constituents are in the Supplementary Materials. Figure 6-3 shows the posterior model probabilities for TSS, NO_x and FRP for the 100 models with highest PMP (Appendix A3, Figure S-27 and Figure S-28 shows other constituents). Red indicates a negative influence and blue a positive influence. The difference in PIP among the two clusters resulted in quite different plausible model structures (models with relatively high posterior model probability) between the two clusters. A stand-out difference among the two clusters was antecedent vegetation cover condition (Ante_NDVI), which tended to be a more important predictor of TSS for Cluster 2, than for Cluster 1 (Figure 6-3[a]). In addition, the plausible models for Cluster 2 were generally more complex (with a greater number of predictors), expect for DOP and EC (Appendix A3, Figure S-27 and Figure S-28).

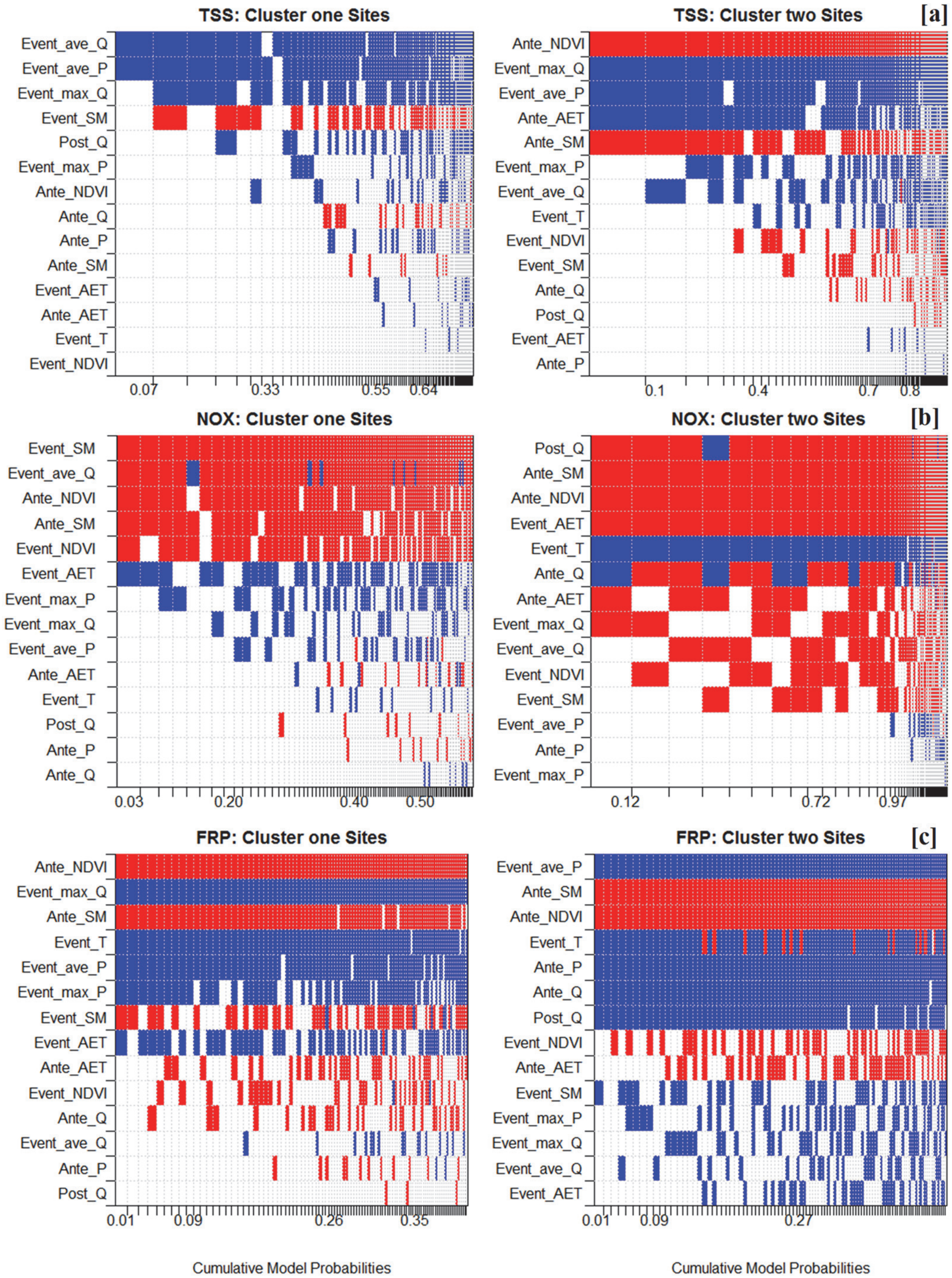

Figure 6-3. Comparison of BMA model coefficients and cumulative model probabilities (only the first 100 models ranked according to the highest probability are shown) between Cluster 1 (left) and Cluster 2 (right) sites for [a] TSS, [b] NO_X and [c] FRP. The order of predictors on the y-axis was ranked based on the posterior inclusion probability. Each column in the heatmap represents the one specific model (ranked from highest model probability) and the width of the column is normalised by the posterior model probability. The colour indicates the direction of the coefficients: red = negative; blue = positive. The coefficient value was averaged across the posterior median value of the site-specific coefficient within each cluster (effect size, $\theta_{n,j}$, in Equation 6-5); the definition of the abbreviations of each predictor on the y-axis are in Table 6-3.

The distribution of posterior model coefficients for the key predictors (Figure 6-4, Appendix A3, Figure S-29 and Figure S-30) further demonstrated the heterogeneity in the effects of event characteristics among different constituents, and across locations. During-event runoff and rainfall tended to have a positive effect on sediment and particulate constituents and, a negative effect on NO_X and EC. In addition, there was strong negative effect of antecedent vegetation condition on the majority of the constituents.

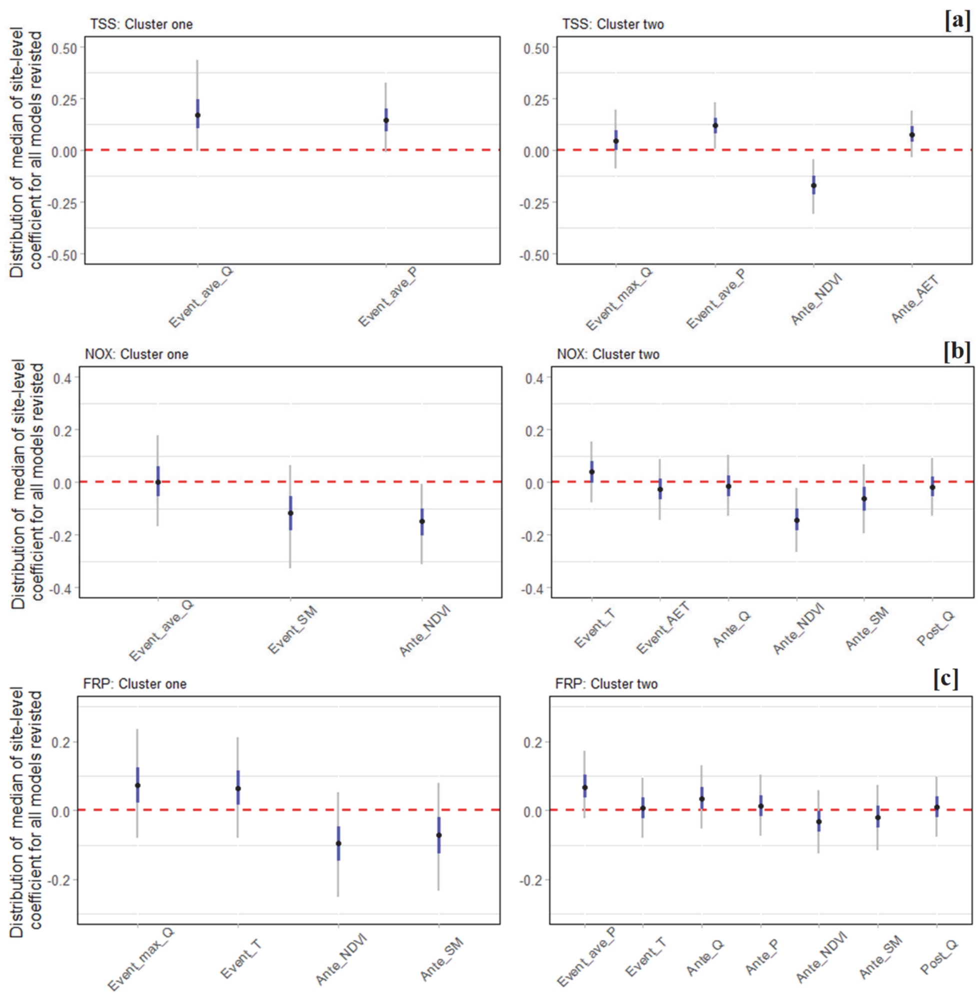

Figure 6-4. Distribution of median of site-level coefficients for all plausible models in BMA for: [a] TSS; [b] NO_X and [c] FRP. Only predictors with PIP > 0.8 are included. For each specific model structure, the coefficient value of a predictor was the median of the site-specific coefficient across all sites (effect size, $\theta_{n,j}$, in Equation 6-5). The distribution of this value thus represents the probability of the model (PMP), as well as variability in the same predictor across different sites; black dots = the median; grey vertical lines = 95% CI; blue coloured vertical lines = 50% CI; the definition of the abbreviation of each predictor on x-axis are in Table 6-3.

The uncertainty in PIP, derived from 1,000 subsampled BMA runs (Figure 6-5, Figure S-31 and Figure S-32) showed that the BMA results were robust for most constituents, except for EC (Figure S-32[c]). Large uncertainty in the PIP for EC was observed, indicating that the BMA results were sensitive to the observations chosen.

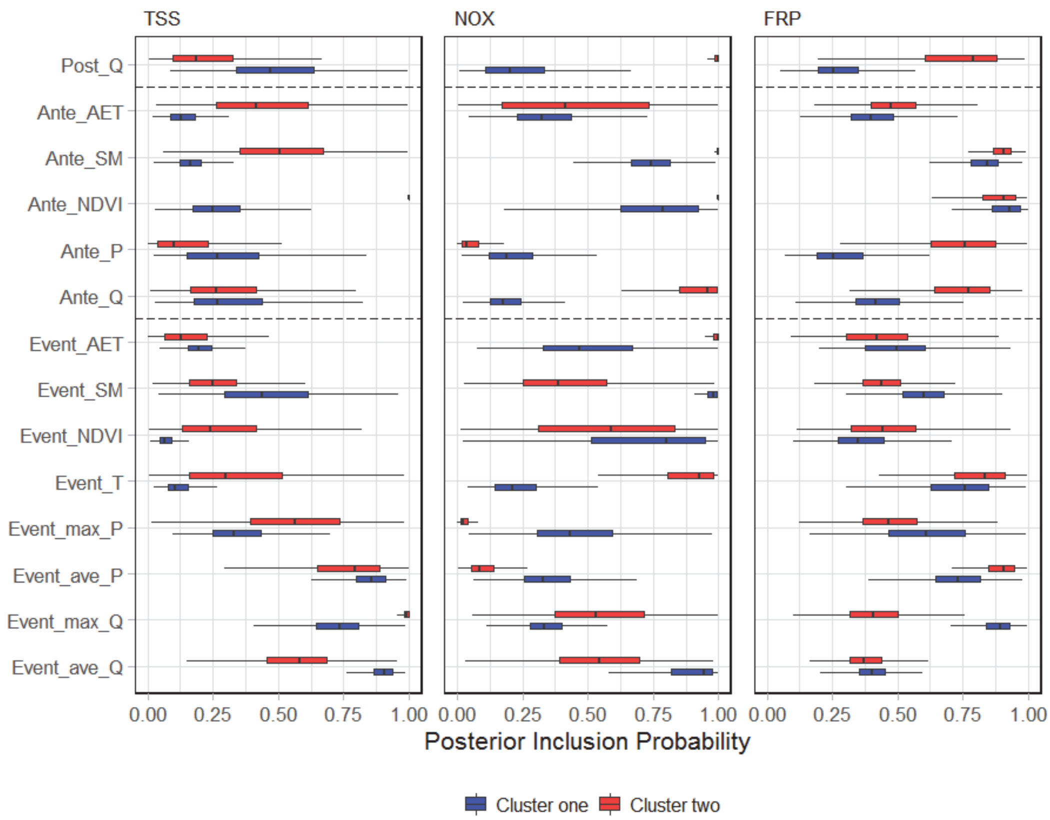

Figure 6-5. The comparisons of the distribution of posterior inclusion probabilities of the individual predictors derived from 1,000 subsampled BMA runs; the boxes are the interquartile ranges (IQR, 25th to 75th percentile), and the whiskers are the ranges between 1.5 IQR of the lower quartile and 1.5 IQR of the higher quartile; the vertical bar = median; blue = Cluster 1; red = Cluster 2; the definition of abbreviation of each predictor on y-axis are in Table 6-3.

6.4.2 Predictive performance

Moderate levels of temporal variability were explained by the BMA framework for the two independent site clusters (Figure 6-6, Figure S-33 and Figure S-34). At the cluster level, the NSE ranged from 0.04 (DOP) to 0.68 (EC) and from 0.34 (NH_4) to 0.64 (NO_X) for Clusters 1 and 2 (the full model columns in Table 6-4), respectively. The comparison of the modelling performance (posterior median of BMA prediction) showed that the modelling framework performed better on the Cluster 2 sites than Cluster 1 (Figure 6-6, red 50% prediction CI – Cluster 2), except for NH_4 and EC (not shown). This was reflected in a better match to the 1:1 line within the 90% prediction CI for Cluster two catchments. It is also worth noting that the prediction interval for EC (Figure S-34[c]) was much wider than the rest of the constituents. Similar results were found in the site-level performance, with the average site-level NSE (Figure 6-7) for the Cluster 2 models typically higher than for Cluster 1 models. The site-specific performance varied across sites, with the largest variation in EC (the NSE for the Cluster 2 result ranged from approximately 0.20 to 0.90). The modelling performance of DOP in the Cluster 1 sites was poor (NSE = 0.04); all candidate covariates had low predictive power, resulting in the poor mixing of chains of the inclusion variable I_n (i.e., posterior I_n was around 0.5). The model residuals were normally distributed (Appendix A3, Figure S-35) and there was no clear heteroscedasticity within the residuals (Figure S-36 to Figure S-44).

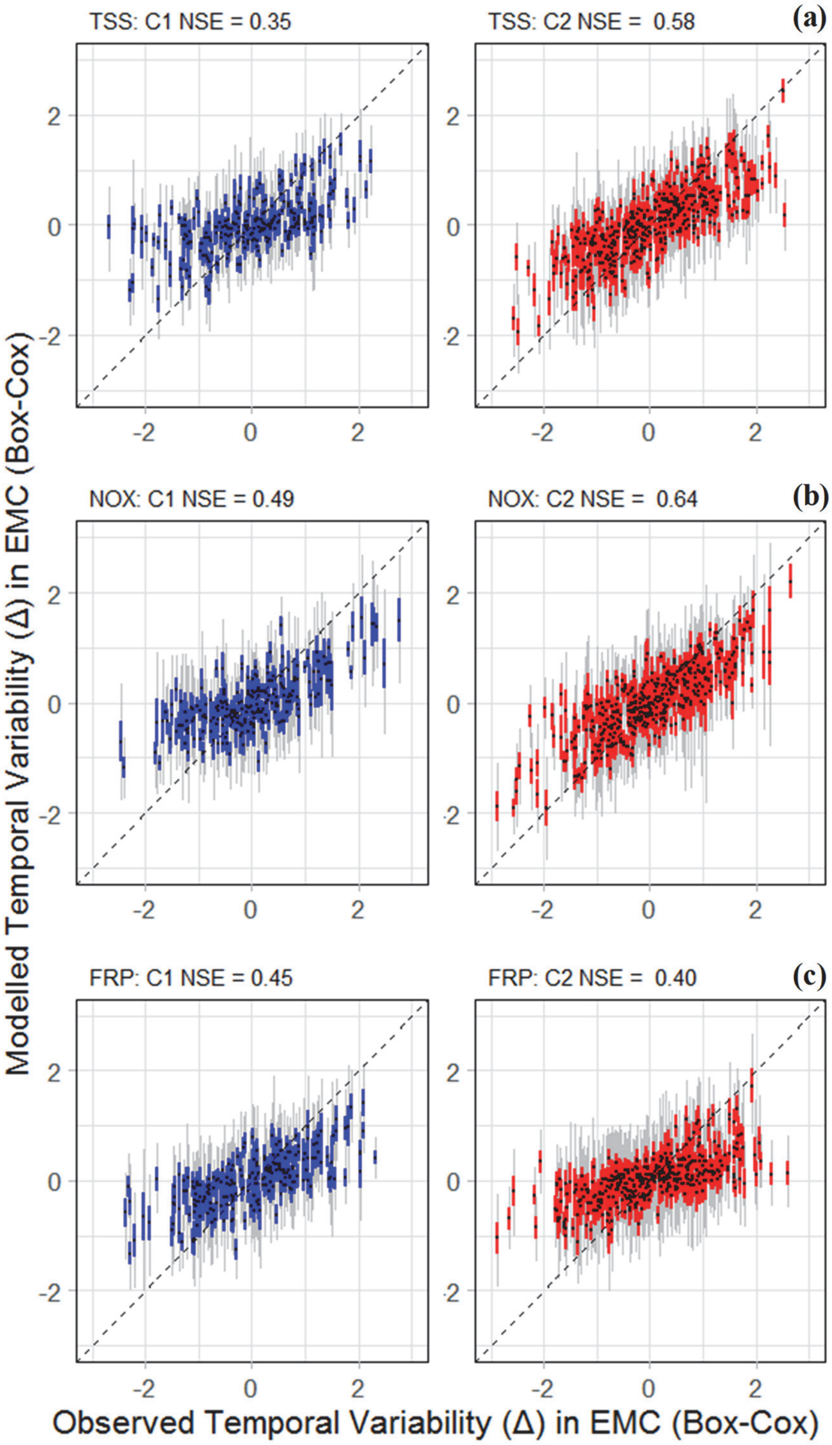

Figure 6-6. Performance of the BMA models of the temporal variability of nine constituents across 32 sites, represented by prediction intervals from BMA and observed Box-Cox EMC across two clusters of sites for: (a) TSS; (b) NO_X; and (c) FRP. Each bar shows a single event and all events at all sites in the cluster are included. The NSE values were calculated based on median predictions. Black dots show prediction median; grey vertical lines show 95% CI; coloured vertical lines show 50% CI; blue is Cluster 1; red is Cluster 2; and dashed black lines are the 1:1 relationship.

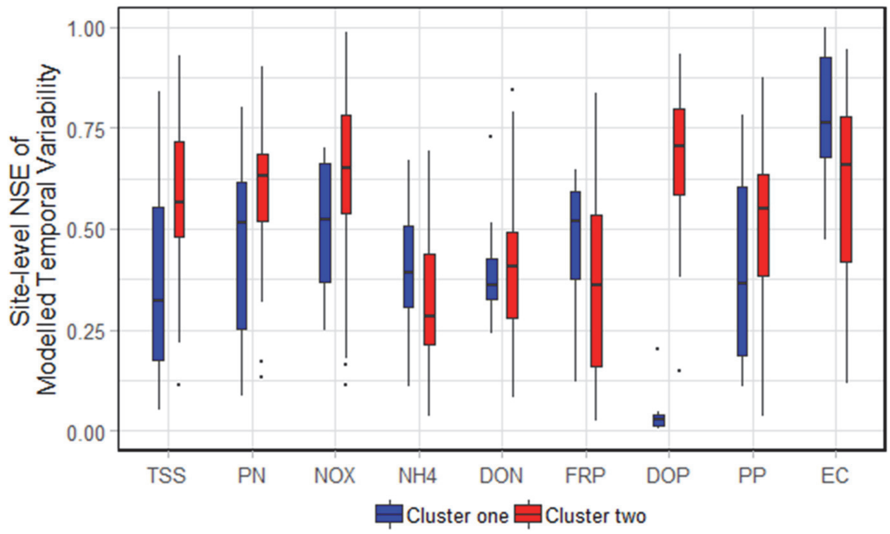

Figure 6-7. Distribution of site-level NSE for modelled the temporal variability of two clusters of sites; the interpretation of boxplot is the same as in Figure 6-5; NSE values were calculated based on site-level predictions of event median EMC; blue is Cluster 1; and red is Cluster 2.

Table 6-4 compares the model performance using rainfall/runoff related predictors only and all candidate predictors (full model). A large increase in NSE was found for most dissolved nutrient species (e.g. NO_X, NH_4, DON, FRP and DOP) for the full model. Notably, for NH_4 in Cluster 1, factors other than rainfall and runoff explained almost all the variability that could be captured by the BMA.

Table 6-4. Comparison between BMA performance using rainfall/runoff predictors only and all candidate predictors (full models).

Constituent	Cluster 1 (NSE)			Cluster 2 (NSE)		
	Rainfall, runoff only	**Full model**	**% change in NSE**	**Rainfall, runoff only**	**Full model**	**% change in NSE**
TSS	0.32	0.35	11	0.42	0.58	38
PN	0.32	0.40	24	0.38	0.59	56
NO_X	0.23	0.49	113	0.32	0.64	101
NH_4	0.00	0.39	/	0.18	0.34	88
DON	0.20	0.37	84	0.20	0.43	117
FRP	0.27	0.45	68	0.26	0.40	56
DOP	0.00	0.04	/	0.22	0.62	181
PP	0.29	0.36	24	0.34	0.51	51
EC	0.41	0.68	66	0.39	0.54	39

6.5 Discussion

6.5.1 Factors influencing temporal variability in stream water quality

6.5.1.1 Runoff and rainfall

Our results demonstrated that runoff and rainfall were important factors in explaining the temporal dynamics of particulate pollutants (i.e. TSS, PN and PP) and dissolved species (e.g., NO_X, DOP and EC) in the GBR catchments. These results accord with the findings of previous studies that have used these variables to understand changes in water quality over time (Letcher et al., 2002; Liu et al., 2008b; McKergow et al., 2003; Schwarz et al., 2006; Tilburg et al., 2015).

Hydrologic and climatic variables (i.e. rainfall and runoff) showed distinct effects on different constituents, as well as different groups of catchments. The positive effect of event runoff and rainfall on sediment and particulate nutrients (i.e., PN, PP) revealed their potential impacts on pollutant mobilisation and transport processes in catchments (Ballantine et al., 2009; Guo et al., 2010b; Heathwaite et al., 2000; Hirsch et al., 2010; Lintern et al., 2018b; Musolff et al., 2015). In contrast, there were negative effects of during-event runoff on NO_X (Cluster 1), DOP (Cluster 2) and EC (both clusters). For NO_X and EC, this was most likely caused by hydrological transport processes; these constituents tend to be transported to receiving rivers via subsurface flows (Kratz et al., 1997; McKergow et al., 2003). For events with relatively low surface runoff, higher NO_X and EC event concentrations could be expected in these catchments, due to a higher fraction of groundwater in surface runoff; that is dilution is important (Clow & Sueker, 2000; Skoulikidis et al., 2006; Young et al., 1996). In addition, for DOP, in-stream biogeochemical cycling was likely to have caused the negative effect of event runoff. In large and dry Cluster 2 catchments, events with low runoff are typically coupled with high temperatures (positive effect of event temperature for DOP Cluster 2, Appendix A3, Figure S-30). Under such circumstance, long residence time and high ambient temperature would enhance P release from sediments, leading to high DOP level in streams (Beutel & Horne, 2018; Verheyen et al., 2015).

Post-event runoff (Post_Q) showed effects on specific constituents (e.g., NOx, FRP and EC). Two alternative reasons might explain this. First, high post-event runoff may be an indicator of large baseflow contribution during the events (Cuomo & Guida, 2016). Therefore, as discussed in the above paragraph, constituents that are likely to be transport through subsurface flows tend to be influenced by amount of runoff after event. Alternatively, it was significantly and positively correlated with other event characteristics and catchment biophysical conditions (e.g., vegetation cover, Appendix A3, Figure S-26). These inter-correlated factors together could have influenced pollutant source, mobilisation and delivery (see discussions below) (Granger et al., 2010; Lintern et al., 2018a).

6.5.1.2 Vegetation cover

Vegetation cover was another driving factor that was found to have influenced water quality dynamics; antecedent NDVI (Ante_NDVI) that covered vegetation conditions three months prior to the event (Table 6-3), was more likely to have been included in the plausible models than event NDVI. This indicated that compared to the vegetation cover during events, vegetation condition before runoff events were more important in determining the temporal variability in water quality. The negative effect of antecedent NDVI on particulate and dissolved nutrients (except DOP) was in line with previous studies that have found that NDVI was negatively correlated with these constituent concentrations in streams (Griffith et al., 2002; Liu et al., 2015; Masocha et al., 2017). An explanation for these results could be that vegetation nutrient assimilation and retention processes consumed nutrients in sediment and waterbodies, and the rate these processes peaked in spring and early summer, typically before the wet season in the GBR catchments (Tabacchi et al., 2000; Uwimana et al., 2018; Vymazal, 2007).

The effect of antecedent NDVI varied among groups of constituents in Clusters 1 and 2. Specifically, it was a key predictor for NO_X, NH_4 and FRP for Cluster one, and almost all constituents for Cluster 2. This may be explained by the contrasting landscapes and climate of these two regions (Liu et al., 2018). In the dense, vegetation-covered catchments in Cluster 1 (i.e., the sites in the Wet Tropics), dissolved inorganic nutrient losses were likely due to more fertile soils (e.g., application of fertiliser on sugarcane) during the growing season (Hunter & Walton, 2008; McKergow et al., 2005a). Furthermore, denser natural vegetation cover (e.g., riparian vegetation and forest) could increase plant uptake and assimilation of dissolved nutrients compared to the sparse vegetation cover in the Dry Tropics (Cluster 2) region. Conversely, among Cluster 2 sites, vegetation coverage showed clear seasonal variation, which was linked closely to the seasonality in rainfall and grazing activity. Sediment and particulate pollutants were likely to be mobilized in grazed catchments (high rate of soil erosion) and delivered to streams via surface runoff (Ballantine et al., 2009; Neil et al., 2002; Turner et al., 2012). The vegetation effect of sediment trapping/retention is important because the sediment was more likely to settle out in larger catchments with longer stream networks (Klapproth & Johnson, 2009; Masocha et al., 2017). More importantly, high vegetation cover tended to mitigate mobilisation of pollutants in catchments, through stabilising the surface soil and such that reduces sediment losses from erosion (Meyer et al., 1997; Rey, 2004; Singh et al., 2008; Zorzal-Almeida et al., 2018).

6.5.1.3 Soil moisture and evapotranspiration

The results showed that soil moisture (SM) and actual evapotranspiration (AET) had a high impact on different constituents, particularly in the Cluster 2 catchments (e.g., antecedent soil moisture [DON and EC], antecedent AET [TSS and EC]). These two variables were inter-correlated and affect the vegetation cover and hydrological cycle (Correll, 1996; Correll & Weller, 1989; Legates et al., 2011). The results indicated that antecedent soil moisture had a negative effect on PN, NO_X, NH_4, DON, DOP and FRP. On one hand, this was expected as antecedent soil moisture was positively correlated with vegetation cover, and high soil moisture tends to reduce soil erosion and increase plant nutrient uptake. It may also be that soil water content affected soil microbial activity, influencing the biogeochemical processes in catchments, such as denitrification (Doran et al., 1988; Doran, 1980; Weier et al., 1993). The rate of denitrification was also enhanced under anoxic conditions, when soil moisture was high (Skopp et al., 1990; Zhu et al., 2018a). On the other hand, higher soil water can be associated with increased shallow subsurface flow and leaching of some constituents such as NO_X (Zhu et al., 2018b). This appears not to occur to a sufficient extent for it to over-ride other impacts of soil moisture. More importantly, antecedent soil moisture is important factor in the generation of runoff, which in turn affects pollutant mobilisation and transport (Schoener & Stone, 2019).

6.5.1.4 Temperature

This study found that average event temperature (Event_T) had a positive effect on NO_X, FRP, and DOP. This may be attributed to the strong negative cross-correlation between temperature and event runoff and antecedent vegetation condition (Appendix A3, Figure S-26). Rainfall during a cooler period might have been associated with more event runoff, resulting in lower event mean concentrations (Section 6.5.1.1). The effect of event temperature can be also attributed to the fact that the higher temperatures could lead to more recent mineralisation of nutrients, increasing readily transportable dissolved nutrient sources (Liu et al., 2017c). This effect might over-ride the effect of uptake of nutrients that is typically enhanced in high temperature (Bernhardt et al.,). In addition, higher event temperature might be associated with higher pre-event temperature, resulting in poor groundcover, potentially lowering the dissolved nutrients losses through plant assimilation/uptake (Section 6.5.1.2) (Muro et al., 2018).

6.5.2 Predicting temporal variations in water quality

The analysis showed that the Bayesian modelling framework offered a useful tool to assess in-stream water quality dynamics. The models were able to explain more of the temporal variation in NO_X and EC than in other constituents. This may have been related to the sources and delivery processes of these two constituents. For instance, temporal changes in NO_X can be well-captured by changes in catchment vegetation cover, which represent the effect of anthropogenic inputs (e.g., agriculture); for EC, large stores in groundwater together with limited geochemical transformation suggested that temporal changes in event concentration of EC could well predicted by the changes in catchment hydroclimatic conditions. In addition,

NO_X and EC tend to be transported in subsurface flow pathways. The dynamics of catchment soil wetness and vegetation cover have been previously linked to hydrological interactions between surface and subsurface flows (Ursino et al., 2004). The incorporation of soil moisture and vegetation cover into the Bayesian modelling framework more readily allowed the description of the main ecohydrological processes of these two constituents. In contrast, model performance for DOP was poor in Cluster 1 catchments, which might potentially be explained by two reasons. First, in the Wet Tropics catchments, DOP concentrations were generally stable, regardless of changes in flow, which can be explained by chemical exchange processes between water and sediment in stream (White et al., 1998). This means that the variability in DOP cannot be captured by the environmental variables considered here. Second, the poor performance could be attributed to the data set having fewer observations of DOP EMCs among Cluster 1 sites. There were only 66 observations, compared to the next lowest number of 167 (EC) among other constituents in the Cluster 1 catchments, which may not be sufficient to full inform the model. This small sample size might have led to outcomes of: 1) poor mixing of MCMC chains for inclusion variables (Figure S-32[a]), where no predictors showed predictive power (high uncertainly in model structure); and 2) the BMA failed to identify the plausible model, since none of the candidate models had enough predictive power to fit the data well (Guthke, 2017; Höge et al., 2019). Continuous DOP monitoring would be required to achieve a better understanding of the factors driving temporal variation in this constituent.

Statistical modelling in hydrology or water quality is affected by uncertainty, only some of which can be characterised within any particular modelling framework (Beck, 1987; Kavetski et al., 2006; Mantovan & Todini, 2006; Renard et al., 2010; Yang et al., 2007). The present study's Bayesian modelling framework incorporated the uncertainties in model selection (between-model), observations and model parameters (within-model) directly into the model predictions (Steel, 2019). This is a more comprehensive characterisation than in studies where model structures are assumed a priori. Reporting of predictive uncertainty of temporal variations in water quality also provided valuable information on the confidence in the averaged predictions. Nevertheless, limitations remain in the BMA approach which are important to understand. One potential issue with BMA is that the posterior model probability could be sensitive to the specification of the parameter prior distribution (Fernandez et al., 2001). Specifying more informative priors on model parameters (i.e., inclusion variable I_n), would have the effect of restricting the set of candidate models (Eicher et al., 2011; Rockey & Temple, 2016). Indeed, several studies have compared different predictive performances of different prior specification of BMA coefficients and found that the choice of prior matters (Bayarri et al., 2012; Eicher et al., 2011; Liang et al., 2008). Future investigation of the sensitivity of prior distributions for BMA coefficients might achieve a reduction in predictive uncertainty and instability in posterior inclusion probabilities.

6.5.3 Management implications

The identification of key drivers of temporal variation in water quality has the potential to inform the catchment water quality management. The results of this study showed that the effects of hydro-climatic drivers and vegetation cover varied among constituents and regions. This allows a catchment manager to identify regions where land management and restoration would have a greater effect on mitigating sediments and nutrients export. The results suggested that, compared to wet catchments, maintaining vegetation ground cover in large dry grazed catchments (e.g., the Burdekin and Fitzroy catchments in Cluster 2) before the wet seasons could be an effective way of reducing sediment losses via erosion processes. Management measures (e.g., establishing woodlands and riparian wetlands and re-vegetation of gully channels on grazing land) tend to stabilise riverbanks and reduce sediment losses from hillslope and gully erosions (Loch, 2000; Sherriff et al., 2016). In addition, catchment-specific management that accounts for temporal variation in catchment hydrological connectivity is required for the control of dissolved nutrients. Dominant flow pathways for dissolved nutrients can vary spatially and temporally. For example, subsurface flow in the Wet Tropics region tends to transmit more dissolved nutrient, because prolonged wet conditions lead to this region more likely to be connected via lateral subsurface flow (Geng et al., 2017; Stieglitz et al., 2003). The enhanced mobilisation of leached dissolved nutrients from intensive cropping (e.g., sugarcane) from perched groundwater should be targeted in these catchments (Melland et al., 2012). Management practices, such as conservation tillage, and adaptation of ‘4R’concept (right source, right rate, right time, right place) for fertiliser application may help to minimise dissolved nitrogen losses (Cestti et al., 2003; Merriman et al., 2009; Snyder, 2017). These results are consistent with current, improved land management practices across the GBR catchments (Brodie et al., 2009; Brodie et al., 2012; Hunter & Walton, 2008; Star et al., 2015).

6.6 Conclusions

This study provides a data-driven understanding of key drivers influencing the temporal variation in water quality. A hierarchical Bayesian model averaging framework was used to identify the key environmental drivers and predict the water quality dynamics at multiple catchments. Results showed that the temporal dynamics of water quality can be predicted well using models considering the combined effects of hydroclimate and vegetation groundcover. The effects of key hydro-climatic and vegetation conditions varied among different constituents, and across regions. This study reinforces the importance of vegetation cover management as one key management response, especially for large grazed catchments. Future investigation could involve the development of a spatio-temporal modelling framework to fully capture the water quality dynamics. More importantly, it has continued to be challenging to prioritise management practices and evaluate the effectiveness of the improved management interventions. Consequently, with more land management surveys and continuous water quality monitoring data available, an extended temporal or spatio-temporal modelling framework could potentially be used to assess if the success of the restoration measures.

Chapter 7 Discussions and Conclusions

In this final chapter, the results of the main chapters are summarized in Section 7.1, and their implications are briefly discussed (Section 7.2). The identified limitations and potential future research to address the limitations are covered in Sections 7.3 and 7.4, respectively.

7.1 Summary of Results

The key tasks to effectively manage instream water quality issues in the GBR catchments are: 1) developing appropriate methods for evaluating long-term, collecting and evaluating large-scale water quality monitoring data; 2) developing suitable modelling tools for predicting water quality have been major tasks for catchment managers. Accordingly, this thesis aimed to achieve the following goals: 1) to better understand the patterns of water quality variation over space; 2) to identify the key factors that determine the spatial and temporal variation in instream water quality, and 3) to predict water quality dynamics at the catchment-scale. To achieve these research objectives, I analysed, modelled and interpreted the water quality monitoring data collected from multiple inland catchments of the Great Barrier Reef, in north-eastern Queensland, Australia. Most of these data were sampled at relatively high temporal resolutions during flow events. This research identified the key factors that influence water quality dynamics, and the implications of these factors for improving future water quality management (see Chapters 4, 5 and 6).

Chapter 4 addressed Research Question 1, which aimed to gain an understanding of underlying spatial patterns in water quality. The investigation applied multivariate analyses on time-averaged constituent concentrations. Results revealed that the study catchments can be grouped into two distinct clusters, which have contrasting patterns in terms of spatial variation in water quality. This was likely due to heterogeneity of the catchment landscape characteristics. The spatial variation in water was closely linked with anthropogenic catchment characteristics (i.e., land use). These results provide useful recommendations for developing future catchment management strategies. For example, large grazing catchments could be targeted to reduce sediments and particulate nutrients in waterways, and key management practices should be adopted to control DIN exported from land use for sugarcane growing. In addition, the results also indicated that dissolved nutrient concentrations are higher within wetter catchments where stream networks are well-developed, suggesting that further research is required to nutrient control in these catchments, such as improved fertiliser management. The results also suggest that the spatial variation in water quality is predictable from key catchment landscape characteristics, which was the objective of Research Question 2.

Chapter 5 investigated the controls and predictability of the spatial variation of event mean concentration of different constituents, via estimating the relative importance of the natural and anthropogenic characteristics. Results from a multi-model inference analysis indicated that in general, natural characteristics in the catchments had strong predictive power when predicting spatial differences in water quality, while land use also has an important impact on dissolved nutrients (e.g., NH_4 and NO_X). The frequentist model averaging framework used predicted average event-mean concentrations well performed and could therefore be used to identify potential hot-spots of water quality concern at ungauged locations.

The key catchment-scale hydroclimatic and environmental factors associated with temporal variation in water quality were explored in Chapter 6. The relative importance of these potential factors was determined using Bayesian hierarchical models and Bayesian multi-model inference. The Bayesian hierarchical modelling framework was able to predict the temporal variation in water quality across multiple catchments. Results indicated that the key factors affecting temporal changes in water quality varied among different constituents and across different catchments. Catchment runoff and rainfall had stronger influences on particulate constituents, while catchment wetness and vegetation cover had more impact on dissolved nutrients and salinity when compared to particulate constituents (e.g., TSS and PN). In addition, in large and dry catchments, antecedent catchment soil moisture and vegetation showed greater influences on dissolved nutrients, indicating the strong effects of catchment hydrological connectively, modulated by vegetation conditions, for pollutant mobilisation and delivery.

In summary, the spatial and temporal variations in water quality during runoff events were well linked with catchment landscape characteristics and time-varying event hydroclimatic and vegetation cover conditions. In this thesis, a comprehensive understanding of spatial and temporal variability in water quality and its association with key controls was successfully achieved, providing valuable information for decision-making in catchment management to reduce the impacts of land-derived pollutants on the GBR.

7.2 Discussion

7.2.1 Differences in inferred controls of water quality 'spatial' variation

The multivariate analyses in Chapter 4 and statistical multi-model inferencing in Chapter 5 both focused on the spatial aspect of the spatio-temporal water quality dynamics. The objectives of these two chapters were to identify the potential factors affecting the time-averaged water quality constituents' concentrations across the GBR catchments. Notably, the influential factors identified from these two chapters differed to some extent. This was due to: 1) different definitions of 'spatial' variation in water quality; and 2) a more extensive set of catchment characteristics being included in Chapter 5.

The spatial variation in water quality used in Chapter 4 was defined as 'time-averaged' concentration; all available samples at each site were used regardless of the flow condition (e.g. event flow or baseflow). However, in Chapter 5, the average flow-weighted concentration across several runoff events was used to characterise the spatial difference of water quality. A comparison between the two derived site-level averages (i.e., spatial difference; Figure 7-1) indicates that the majority of constituents had similar time-averaged concentrations and average EMC. One exception was DOP. The higher time-averaged concentration of DOP compared with average EMC is an indication of higher DOP concentrations during baseflow.

Compared to other constituents, DOP can be more variable and lower during events due to its high reactivity (e.g., phosphorus enrichment by plant productivity) and source-limited nature (Chow et al., 2017; Chow et al., 2013; Qualls & Richardson, 2003).

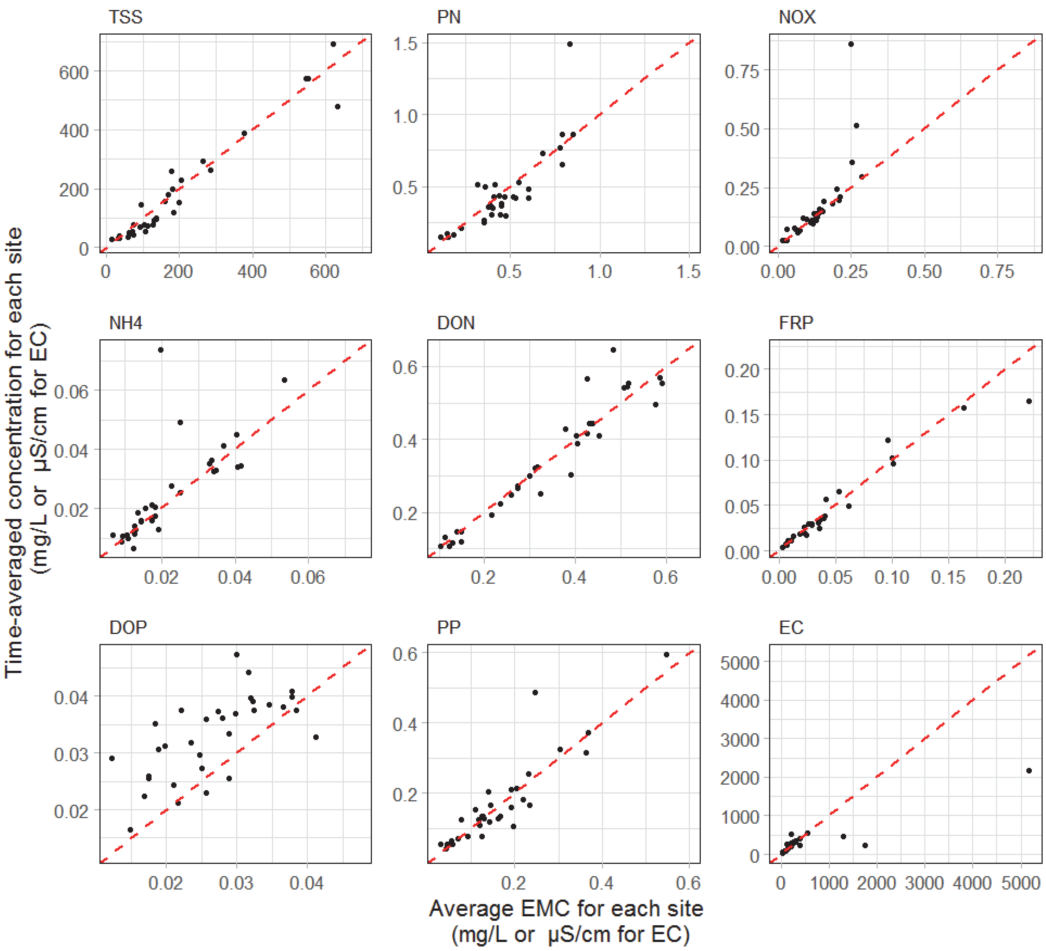

Figure 7-1. Scatter plot of relationship between site-level average EMC and time-averaged concentration for nine constituents across the 32 GBR catchments; red dashed line =1:1 line; TSS=total suspended solids; PN=particulate nitrogen; NO_X=oxidized nitrogen; NH_4=ammonium nitrogen; DON=dissolved organic nitrogen; FRP=filterable reactive phosphorus; DOP=dissolved organic phosphorus; PP=particulate phosphorus; EC=electrical conductivity.

In Chapter 5, additional catchment characteristics were considered in the investigation, and the relative importance of catchment landscape characteristics was further evaluated. The approaches adopted in Chapter 5 also differentiated between the less informative characteristics where many potential explanatory factors showed high cross-correlation, whereas Chapter 4 did not. This resulted in differences in the detected key controls on spatial variation in stream water quality for some constituents between these two chapters. The differences also resulted from the fact that Chapter 4 handled the water quality and catchment characteristics independently and linked them from a multivariate perspective; while in Chapter 5, the spatial variation in water quality was explained by a set of plausible statistical models. The results of both chapters, however, indicate that the underlying catchment controls on spatial differences in water quality varied among different constituents. The natural characteristics of the catchments, especially climate and geology, were important factors for a majority of the constituents, while anthropogenic characteristics, such as catchment land use (e.g., sugarcane) were identified as key factors affecting the concentrations of dissolved nitrogen.

7.2.2 Decomposition of the total variation and modelling performance

Chapters 5 and 6 addressed RQs 2 and 3, respectively. In these two chapters, the total variance in measured EMC of different constituents are decomposed into spatial (Chapter 5, deviation of site-level average from the global mean, Equation 7-1) and temporal (Chapter 6, deviation of individual EMC from the site-level average, Equation 7-2) components, which are defined as follows.

$$\sigma^2_{spatial} = \sum_{j=1}\sum_{i=1}(\overline{EMC_j} - \overline{EMC})^2 \qquad \text{Equation 7-1}$$

$$\sigma^2_{temporal} = \sum_{j=1}\sum_{i=1}(EMC_{i,j} - \overline{EMC_j})^2 \qquad \text{Equation 7-2}$$

where, $EMC_{i,j}$ is event-mean concentration for i^{th} event at j^{th} catchment, $\overline{EMC_j}$ is the averaged EMC at j^{th} catchment and $\overline{EMC}$ is the global averaged EMC across all catchments.

The partitioning of these two components (Figure 7-2) indicates that spatial variation accounts for a larger proportion of total variability for most constituents (except for DOP). This indicates that if the spatial variation can be well predicted, the dynamics of constituents (e.g., DON, FRP and EC) are more likely to be captured by a spatio-temporal modelling framework.

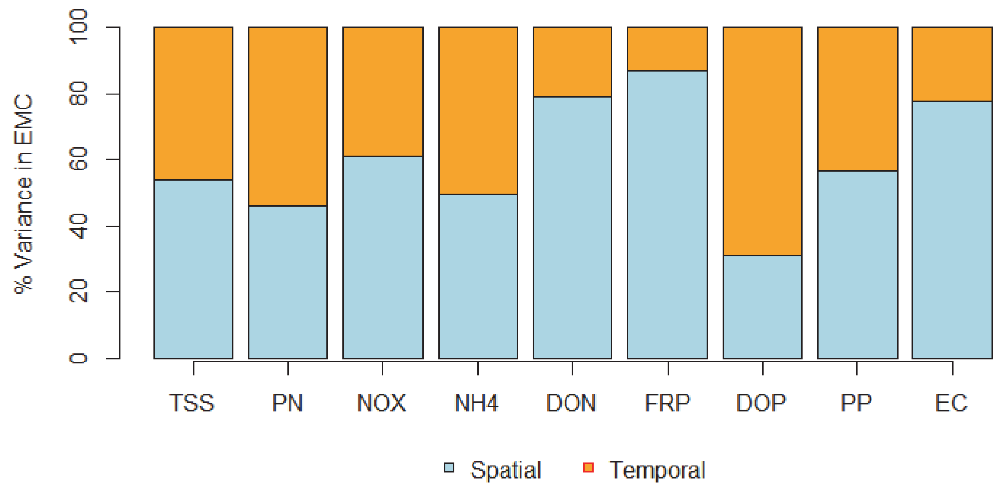

Figure 7-2. Variance decomposition of EMCs. The spatial component is derived from the deviation of site-level average EMC and global averaged EMC for specific constituents. The temporal component is derived from the deviation of individual EMC and site-level average EMC for specific constituents; the variance was estimated based on Box-Cox transformed EMCs; TSS=total suspended solids; PN=particulate nitrogen; NO_X=oxidized nitrogen; NH_4=ammonium nitrogen; DON=dissolved organic nitrogen; FRP=filterable reactive phosphorus; DOP=dissolved organic phosphorus; PP=particulate phosphorus; EC=electrical conductivity.

The predictive spatial and temporal water quality models developed in this research provided an indication of key spatial and temporal controls on decomposed water quality dynamics, as well as a potential modelling framework to integrate these two levels of variability. A comparison of modelling performance on the spatial and temporal variations (Table 7-1) shows that spatial models were performing better than the temporal models for all constituents. In addition, spatial models for the dissolved species (e.g., NO_X and DON) performed better. Among these dissolved constituents, the spatial and temporal variations of NO_X and EC were predicted with high accuracy. The results indicate that: 1) the spatial part of the total variability in water quality is easier to be captured compared to the temporal counterpart; and 2) the spatial and temporal statistical models used in this research may be able to capture the dynamics of constituents better where subsurface flow is the main transport pathway.

Table 7-1. Modelling performance (NSE) on spatial and temporal variations of nine water quality constituents.

Constituent	NSE of spatial models	NSE of temporal models	
		Cluster 1	Cluster 2
TSS	0.75	0.35	0.58

PN	0.64	0.40	0.59
NO_X	0.83	0.49	0.64
NH_4	0.89	0.39	0.34
DON	0.98	0.37	0.43
FRP	0.95	0.45	0.40
DOP	0.71	0.04	0.62
PP	0.79	0.36	0.51
EC	0.87	0.68	0.54

Note. Results are retrieved from Chapters 5 and 6.

7.2.3 Comparison between model selection approaches

As identified from the literature review in Chapter 2, a major limitation of the existing statistical modelling of catchment water quality is that it does not account for the uncertainty arising from choosing different models. Ignoring the issue of uncertainty from model selection and relying on a single model structure might result in misleading conclusions or overconfidence in the results. In this research, both frequentist model averaging (FMA in Chapter 5) and Bayesian model averaging (BMA in Chapter 6) approaches were adopted to better quantify the uncertainty arising from model selection. There has been active debate on the adequacy of FMA and BMA (Amini & Parmeter, 2012; Hjort & Claeskens, 2003; Raftery & Zheng, 2003; Steel, 2019). In this research, FMA was found to be time consuming when the number of potential covariates was large. As such, to reduce the computational demand, a two-round exhaustive search approach was used (Chapter 5). BMA was more effective and flexible in incorporating model selection uncertainty. BMA application also involved direct inferences on the posterior inclusion probability for individual predictor variables, as well as model probability. This application was relatively straightforward compared to FMA. However, it has been recommended that the assumption of the prior distribution of parameters and sensitivity of the prior distribution on the resulting inferences needs to be considered (Höge et al., 2019; Steel, 2019). Considering the application and the objectives of the investigations, future research could focus on methods to improve the efficacy and efficiency of FMA, as well as robust prior specification of model parameters in BMA.

7.2.4 Implications for future water quality management

In response to the water quality deterioration in the GBR catchments, Australian and Queensland governments have introduced policies designed to control the pollutant loads and protect the coastal aquatic ecosystems. A joint Queensland and Australian government initiative (Reef Rescue Plan, see Department of Premiers and Cabinet (2009) and State of Queensland (2013)) has provided a substantial amount of incentives to encourage famers to change land management practices and to adopt Best Management Practices (BMP) (Schaffelke et al., 2009). Specific regulations have been developed for farmers in terms of adopting improved agricultural management practices (Thorburn & Wilkinson, 2013). The current improved management practices have focused on two main industries: 1) sugarcane for dissolved inorganic nitrogen; and 2) grazing for sediment (Beher et al., 2016; Carroll et al., 2012; Star et al., 2017; Star et al., 2018). These working hypotheses and the associated management prioritization are based on previous conceptual understanding of the effect of BMP on water quality dynamics (Prove et al., 1995; Tosakana et al., 2010) and physically-based water quality modelling results (e.g., Source Catchments) (Waterhouse et al., 2017; Waters et al., 2014). However, despite extensive investment in BMP adoption, the progress has been slow so far (Star et al., 2018). The validity of these working hypotheses is important for evaluation of the current BMP and development of the future management strategies.

The results from this research reinforced the working hypotheses that are currently used to design and prioritise conservation practices. First, the spatial modelling results indicated that the natural environmental factors of catchments (e.g., climate and geology) were the controlling mechanisms that determine the spatial variation of the majority of the constituent, and the land use (e.g., grazing and sugarcane) was largely affecting spatial variations in nutrients and salts. The effective water quality management strategies rely on both understanding of effect of natural and anthropogenic characteristics in catchments on the spatial variation in water quality. This understanding could also improve the ability to identify water quality hotspots, where catchments might experience large pollutant loads or higher concentrations during events.

Second, from a temporal perspective, catchment ground cover and wetness prior to runoff events were two important factors that influenced instream sediment and nutrient event concentrations. This indicates that maintaining good vegetation cover in dry inland catchments, especially during the dry season could help to reduce sediment concentrations in the GBR rivers, which also supported the existing management options (Kroon et al., 2016). As such, management measures could be adopted in these dry catchments to maintain this good vegetation cover and reduce erosion. In addition, hydrological connectivity in the catchments was of great significance in determining temporal dynamics of dissolved nutrient species in coastal catchments (e.g., the Wet Tropics and Mackay-Whitsunday regions). This was found to be linked to the mobilisation of leached dissolved nutrients from intensive cropping (e.g., sugarcane) from perched groundwater. This also indicated that nutrient-rich runoff from fertiliser application could be targeted in these coastal catchments.

In addition to supporting the existing working hypotheses, the results raised new working hypotheses that could be tested in future development of BMP. For instance, these hypotheses could include:1) compared to the conventional landuse-focused prioritization of management, a comprehensive evaluation of relative effects of land uses and catchment natural characteristics will result in a better water quality at the end of catchments; and 2) taking the time-varying environmental factors (e.g., land cover and catchment wetness prior to wet season) into account will lead to improvement in water quality and reduction in pollutant loads during flow events.

7.3 Limitations and Future Research Directions

7.3.1 Transferability

This research was limited to catchments in the north-eastern part of Queensland, Australia. Even though the study catchments featured diverse landscapes (e.g., tropical as well as dry inland catchments) (Bell, 2001; Gilbert & Brodie, 2001), there is still an issue of whether the understanding gained in this research could be transferred to other catchments in Australia and other parts of the world. The controlling factors driving the changes in water quality might vary catchment by catchment beyond the ranges examined in this research. These differences in catchment processes could be attributed to: 1) different baseline hydroclimatic conditions and ecosystem habitats (Aubert et al., 2013; Nilsson & Malm-Renöfält, 2008); and 2) different processes (e.g., large floods or prolonged drought events) that lead to trends and changes in water quality conditions (Elchyshyn et al., 2018; Li et al., 2018a; Richards & Baker, 2002; Tarasova et al., 2018). For example, in the Lower Murray River catchments in South Australia, frequent and intense hydrological droughts and extreme low flows have led to a significant increase in salinity in both rivers and lakes (Kingsford et al., 2011; Mosley et al., 2012). The hydrological condition could become a more predominant factor in those catchments compared to the catchments considered in this research. In northern Australia, the occurrence and intensity of bushfires have also influenced soil erosion and biogeochemical cycling of nutrients (Andersen et al., 1998; Townsend & Douglas, 2000). Therefore, the findings from this research should be interpreted with caution, and the local geographic conditions of any new application should be taken into consideration. Nevertheless, results from this thesis are likely to be transferable to other tropical regions with a similar climate and land uses, such as the northeast of Brazil (de Arruda-Santos et al., 2018; Maciel et al., 2015), and the eastern coastal region of India (Damodharan & Reddy, 2012; Govindaraj et al., 2011), where understanding of water quality dynamics is lacking in these tropical regions.

Inclusion of more case study catchments across Australia and other parts of the world would greatly increase the applicability of the modelling framework in this research. In particular, the inclusion of different climatic zones would enhance the transferability of the modelling framework presented here. The potential selection of catchments depends on the availability of water quality monitoring data and geospatial data. Ideally, if such data are available for several case study catchments within each state in Australia, a national water quality modelling framework could be established.

7.3.2 Sources of pollution

Diffuse pollution from agricultural activities was the focus of this research, and the effects of other sources of pollution were not considered due to limited data availability. This might lead to bias in the results identifying the key controls on the sources of pollution. For example, atmospheric deposition has been identified as a significant contributor of nitrogen enrichment to estuarine/coastal waters (Johnson & Lindberg, 2013; Paerl et al., 2002; Prospero et al., 1996), as well as inland catchments (Jassby et al., 1994; Johnson & Lindberg, 2013; Lohse et al., 2008). In the context of the GBR catchments, Packett (2017) estimated that approximately 30% of the long-term average annual dissolved inorganic nitrogen was likely to originate from precipitation. In addition, contributions from point sources (e.g. discharges from coal mining sites and waste water treatment plants (WWTPs)) were not included in the current analyses. Historically, the development of the coal mining industry in the GBR catchments has resulted in an elevated level of salinity in streams (Grech et al., 2016; Hughes et al., 2015; Prosser, 2011).

To improve the understanding of nutrient sources and dynamics in the GBR catchments, further investigation is need to better understand: 1) the interaction between anthropogenic emissions; 2) rate of atmospheric deposition, and 3) the factors affecting these processes. Point source pollution from human activities could also be considered in future development of the modelling structure used in this research. Collecting more information, such as timing and volume of effluent from WWTPs, could be a potential starting point to investigate the model performance when this point source information is included. Most effluent released into waterways from WWTPs, and annual volume and load of sewage treatment plants for each of six NRMs have been estimated by the Department of Environment and Science (Queensland Government, 2019). In addition, other statistical approaches might be useful when exploring the contribution of point sources. For instance, Walsh et al. (2017) used a random forest approach to investigate the effect of WWTPs on the spatial distribution of sediment and particulate pollutants in an estuarine catchment, in Narragansett Bay, Rhode Island, USA.

7.3.3 Consideration of temporal changes in land uses and land management

The current modelling did not consider the recent land management changes including programs to incentivise Best Management Practices (BMP). In the GBR catchments, a management practice rating framework and associated water quality risk framework for each industry (sugarcane, cropping and grazing) has been developed (Waters et al., 2013). This framework is used to classify farming practices within a given landscape (from A – Aspirational Best Practice/Low Risk to D – Traditional Practice/High Risk), based on resulting water quality improvements for sediment, nutrient and pesticide management (Drewry et al., 2008; Rolfe & Harvey, 2017; State of Queensland, 2013). Since 2013, a detailed paddock-scale survey has been carried out annually, and the benchmarks have been developed for each agricultural sector within each major catchment (McCloskey et al., 2017; van Grieken et al., 2019). In this thesis, the effectiveness of BMP was not evaluated because of: 1) the relatively short period of the survey period (from 2013 to 2016); 2) the challenges in data interpretation related to variable benchmark or baseline conditions prior to the implementation of BMP; and 3) the time-lag between changes in catchment management practice and any resultant changes in water quality (Ilampooranan et al., 2019; Meals et al., 2010; Melland et al., 2018). As improved data on land management becomes available, the modelling frameworks developed here should be extended to include the effects of BMP implementation.

The effect of BMP can be explored by both statistical (Geng et al., 2015; Qi et al., 2018; Steinman et al., 2018) and physically-based approaches (Bracmort et al., 2006; Chen et al., 2016a; Dong et al., 2018; Santhi et al., 2006). The modelling framework developed in this thesis will be useful to examine the effectiveness of BMP once long-term data/information on BMP, as well as water quality monitoring data are collected in the GBR catchments.

7.3.4 Scale consideration

The effect of catchment landscape characteristics on stream water quality is scale-dependent (Buck et al., 2004; Hunsaker & Levine, 1995; Pratt & Chang, 2012; Uriarte et al., 2011). In this research, the relationship between landscape characteristics and water quality responses was investigated at the catchment scale. However, the effect of landscape structures on riverine water quality might vary at different scales. This might result in difficulties in interpretation of the results from this research, due to a lack of mechanistic understanding at local scale. For instance, studies have identified that catchment scale land uses can be better predictors when predicting nutrient levels (de Mello et al., 2018; Johnson et al., 1997; Liu et al., 2017a; Roth et al., 1996; Sponseller et al., 2001). However, at the riparian buffer or stream corridor scale, land use, geology and topography information can provide higher modelling strengths for sediment and nutrient species (Basnyat et al., 1999; Mainali & Chang, 2018; Shi et al., 2017). In the spatial modelling of this research, catchment area was included as a potential predictor. This was not a strong predictor of spatial variability in water quality and as such there did not seem to have a strong scale effect. However, there could be some scale effects at finer scales. Further investigation of the scale effect on water quality responses in the GBR catchments would provide more informative evidence on the effectiveness of management practices, such as riparian restoration (Collins et al., 2013).

7.3.5 Integrated spatio-temporal water quality modelling

The spatial and temporal water quality models were developed separately in this research. This restricts the application of the current modelling framework to either assessing spatial variability (e.g., identifying water quality at unmonitored sites) or to temporal variation at monitoring sites included in the modelling. The reason why these two parts have not been combined is that the limited number of observations (i.e. events has not been monitored) thus fewer independent events to evaluate the integrated modelling framework. This would be overcome once more recent monitoring record to be included, thus enabling fully predicting the water quality dynamics using an integrated modelling framework. The modelling cannot be applied to simultaneously understand both spatial and temporal responses in water quality, for example, for temporal variability at unmonitored sites. However, the modelling framework discussed in Chapters 5 and 6 could be further combined, with the observed site-level averaged component (i.e., spatial variability) outlined in Chapter 6 being modelled by the key catchment characteristics identified in Chapter 5. This would allow an enhanced explanation of the spatial and temporal variability in water quality using an integrated modelling framework. This approach could potentially be used to simulate event mean concentrations in ungauged locations. In addition, the impact of hydroclimatic and vegetation variables on the relationship between catchment characteristics and water quality could be further investigated as part of this integrated framework. This relationship would be informative when estimating event mean concentrations for ungauged catchments using the key catchment landscape characteristics, as well as the key temporal environmental factors (e.g., discharge, soil moisture, rainfall and vegetation cover).

7.4 Key Contributions and Conclusions

Despite the limitations identified in the previous section, there are several key contributions derived from this thesis, which advance our understanding of water quality dynamics at large scales. These include:

- An enhanced understanding of the spatial pattern of water quality and its linkage with catchment landscape characteristics. By comparing spatial differences in water quality and catchment landscape characteristics, two groups of catchments among a set of study catchments were found. Cluster one sites had lower time-averaged concentrations (expect for NO_X), which were situated in wet, sugarcane predominantly grown regions; while, Cluster two sites had relatively higher average concentrations with considerable grazing land use. This categorization reflected the main differences in water quality across space and the potential catchment characteristics leading to these differences;

- A modelling framework to model the spatial variability in water quality and identification of the key controls affecting the spatial variability in water quality. This framework was able to compare the relative importance of catchment natural and anthropogenic characteristics. It also accounted for the model selection uncertainty that has been rarely considered in the previous statistical water quality modelling studies.
- An enhanced understanding that catchment natural characteristics were controlling factors in statistically modelling the spatial variability in sediments and particulate nutrients, while catchment anthropogenic characteristics (i.e., land use) are more important factors for dissolved nutrients species. These contrasting findings provided enhanced understanding of differences in constituents' sources, mobilisation and delivery within catchments;
- A Bayesian modelling framework to model temporal variabilities in stream water quality and identification of the key temporal environmental factors affecting temporal variability in water quality across two clusters of sites. The ability to capture the water quality dynamics across multiple locations over large-scale catchments was one of appealing features of this framework.
- Demonstration of how the key temporal controls varied between two clusters of sites, as well as between different constituents. In large and dry catchments, vegetation cover had more profound effect in reducing EMCs of sediment and nutrients, compared to wet and small catchments. Overall, the catchment ground cover condition and soil moisture prior to runoff events were of great importance in determining the temporal change in event concentration. The spatial pattern of water quality responses affected the key controls on temporal variation in stream water quality.

Surface water quality has typically been evaluated and managed at the catchment scale. Accounting for the key controls on spatial and temporal variations in water quality potentially improves estimations of where and when the water quality dynamics pose detrimental impacts on aquatic ecosystems and public health, thereby supporting effective catchment water quality management. This thesis developed a novel water quality modelling framework, which is a useful tool for catchment managers to evaluate water quality dynamics under future changing climates and land uses.

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Appendix

A1. Supplementary Materials for Chapter 4

Table S-1. Description of each selected station

No.	Region	Catchment	Site ID	River and site name	Monitored surface area / km^2	% of catchment Monitored
1	Cape York	Normanby	105107A	Normanby River at Kalpowar Crossing	12,934	53.0%
2	Wet tropics	Barron	110001D	Barron River at Myola	1,945	88.9%
3		Barron	110002A	Barron River at Mareeba	836	38.2%
4		Barron	110003A	Barron River at Picnic Crossing	228	10.4%
5		Mulgrave-Russel	1110056	Mulgrave River at Deeral	785	39.6%
6		Mulgrave-Russel	1111019	Russell River at East Russell	524	26.4%
7		Johnstone	1120049	North Johnstone River at Old Bruce Hwy Bridge (Goondi)	959	100.0%
8		Johnstone	112004A	North Johnstone River at Tung Oil	925	100.0%
9		Johnstone	112101B	South Johnstone River at Upstream Central Mill	400	43.2%
10		Tully	113006A	Tully River at Euramo	1,450	100.0%
11		Tully	113015A	Tully River at Tully Gorge National Park	482	33.2%
12		Herbert	116001F	Herbert River at Ingham	8,581	87.2%
13	Burdekin	Haughton	119101A	Barratta Creek at Northcote	753	18.6%
14		Burdekin	120001A	Burdekin River at Home Hill	129,939	99.9%
15		Burdekin	120002C	Burdekin River at Sellheim	36,290	27.9%
16		Burdekin	120301B	Belyando River at Gregory Development Rd.	35,410	27.2%
17		Burdekin	120302B	Cape River at Taemas	16,070	12.4%

18		Burdekin	120310A	Suttor River at Bowen Developmental Road	10,760	8.3%
19	Mackay Whitsunday	O'Connell	124001B	O'Connell River at Stafford's Crossing	342	40.2%
20		O'Connell	1240062	O'Connell River at Caravan Park	825	97.1%
21		Pioneer	125013A	Pioneer River at Dumbleton Pump Station	1485	94.5%
22		Plane	126001A	Sandy Creek at Homebush	326	12.8%
23	Fitzroy	Fitzroy	1300000	Fitzroy River at Rockhampton	139,159	97.6%
24		Fitzroy	130206A	Theresa Creek at Gregory Highway	8,485	6.0%
25		Fitzroy	130302A	Dawson River at Taroom	15,850	11.1%
26		Fitzroy	130504B	Comet River at Comet Weir	16,460	11.5%
27	Burnett Mary	Burnett	136002D	Burnett River at Mt Lawless	29,360	88.4%
28		Burnett	136004A	Jones Weir HW	21,700	65.3%
29		Burnett	136014A	Burnett River at Ben Anderson Barrage Head Water	32,891	99.0%
30		Burnett	136094A	Burnett River at Jones Weir (TW)	21,700	65.3%
31		Burnett	136106A	Burnett River at Eidsvold	7,117	21.4%
32		Mary	138014A	Mary River at Home Park	6,845	72.3%

Table S-2. Statistical summaries of different constituents for each site (n = total number of samples; μ ± σ = mean ± standard deviation)

Site ID	TSS		PN		NO_X		NH_4		DON	
	n	μ ± σ (mg/L)	n	μ ± σ (mg/L)	n	μ ± σ (mg/L)	n	μ ± σ (mg/L)	n	μ ± σ (mg/L)
105107A	299	33±28	219	0.15±0.081	261	0.27±0.11	265	0.023±0.02	253	0.016±0.011
110001D	645	158±183	569	0.53±0.58	623	0.32±0.11	622	0.071±0.061	606	0.014±0.011
110002A	71	53±81	61	0.25±0.31	71	0.25±0.12	71	0.12±0.092	70	0.018±0.048
110003A	375	93±100	339	0.37±0.33	356	0.3±0.09	380	0.18±0.07	379	0.025±0.017
1110056	262	30±49	236	0.17±0.2	258	0.15±0.073	275	0.15±0.12	273	0.018±0.016
1111019	299	27±32	225	0.15±0.13	267	0.13±0.054	277	0.19±0.14	278	0.02±0.03
1120049	176	43±70	150	0.31±0.4	175	0.11±0.047	185	0.14±0.06	185	0.011±0.0065

112004A	166	52±78	151	0.3±0.38	162	0.11±0.05	168	0.14±0.056	163	0.0067±0.0036
112101B	511	74±110	447	0.42±0.57	490	0.12±0.061	516	0.15±0.071	508	0.0086±0.0062
113006A	1441	39±40	1185	0.17±0.15	1340	0.15±0.067	1390	0.24±0.18	1372	0.013±0.025
113015A	445	35±60	346	0.3±0.46	415	0.12±0.052	428	0.094±0.081	420	0.011±0.011
116001F	436	50±63	360	0.21±0.19	425	0.19±0.1	432	0.19±0.23	435	0.02±0.041
119101A	766	147±488	618	0.51±0.63	660	0.65±0.36	682	0.86±2	674	0.074±0.22
120001A	461	265±413	430	0.44±0.5	459	0.25±0.14	468	0.11±0.1	433	0.011±0.014
120002C	200	478±591	183	0.65±0.71	197	0.22±0.07	198	0.068±0.085	196	0.0098±0.013
120301B	443	257±342	265	0.5±0.53	266	0.44±0.1	262	0.023±0.044	292	0.016±0.023
120302B	372	228±269	302	0.51±0.5	309	0.32±0.088	255	0.026±0.044	321	0.011±0.02
120310A	181	198±234	112	0.43±0.24	116	0.55±0.19	118	0.07±0.19	122	0.016±0.017
124001B	50	97±112	53	0.26±0.24	59	0.3±0.18	60	0.076±0.068	57	0.013±0.011
1240062	132	117±143	134	0.48±0.45	139	0.39±0.15	140	0.12±0.14	137	0.063±0.087
125013A	740	101±157	687	0.42±0.57	692	0.27±0.13	709	0.21±0.25	703	0.045±0.046
126001A	394	77±113	389	0.43±0.47	401	0.56±0.31	405	0.51±0.74	401	0.049±0.076
1300000	307	178±170	280	0.36±0.23	285	0.43±0.18	293	0.14±0.11	295	0.021±0.03
130206A	99	573±785	89	0.77±0.69	88	0.41±0.13	85	0.36±1.6	90	0.013±0.011
130302A	155	388±313	121	0.86±0.45	128	0.57±0.16	156	0.16±0.16	155	0.035±0.041
130504B	123	691±734	116	0.86±0.82	116	0.42±0.13	116	0.12±0.12	120	0.027±0.05
136002D	286	575±1921	275	1.5±2.6	274	0.54±0.17	271	0.059±0.06	291	0.033±0.035
136004A	184	293±335	185	0.73±0.56	181	0.55±0.1	182	0.11±0.084	184	0.041±0.033
136014A	455	77±156	419	0.37±0.5	437	0.44±0.12	417	0.1±0.13	419	0.034±0.041
136094A	71	77±143	69	0.35±0.29	71	0.5±0.19	64	0.063±0.075	68	0.036±0.036
136106A	194	69±62	171	0.38±0.2	196	0.54±0.15	195	0.12±0.09	196	0.034±0.03
138014A	233	153±162	218	0.43±0.31	225	0.41±0.13	232	0.29±0.27	232	0.032±0.025

Table S-2. **(Continued)** Statistical summaries of different constituents for each site (n = total number of samples; μ ± σ = mean ± standard deviation)

Site ID	FRP		DOP		PP		EC	
	n	μ ± σ (mg/L)	n	μ ± σ (mg/L)	n	μ ± σ (mg/L)	n	μ ± σ (μS/cm)
105107A	228	0.0065±0.0066	75	0.036±0.034	229	0.041±0.028	266	92.39±39.74
110001D	594	0.011±0.0089	179	0.026±0.027	528	0.13±0.12	533	77.56±30.55
110002A	71	0.025±0.017	21	0.035±0.071	63	0.077±0.09	67	96.27±26.62
110003A	380	0.016±0.012	219	0.022±0.026	339	0.18±0.16	385	55.63±14.79
1110056	268	0.0094±0.007	10	0.029±0.013	151	0.056±0.04	169	462.9±2666
1111019	260	0.0042±0.002	4	0.037±0.029	150	0.055±0.042	260	240.8±1503
1120049	180	0.0061±0.0027	7	0.024±0.0079	126	0.13±0.16	145	44.77±8.891
112004A	168	0.0078±0.0024	47	0.026±0.025	134	0.11±0.13	168	41.44±10.57
112101B	516	0.011±0.0044	90	0.027±0.028	412	0.17±0.23	319	43.15±9.037
113006A	1248	0.0064±0.0054	164	0.031±0.028	884	0.054±0.042	992	37.06±8.774
113015A	320	0.0034±0.0024	33	0.032±0.022	159	0.077±0.1	218	29.27±3.804
116001F	394	0.0074±0.0067	53	0.038±0.031	245	0.064±0.044	450	72.7±20.39
119101A	677	0.065±0.045	388	0.038±0.05	619	0.12±0.12	871	237.4±171.9
120001A	450	0.028±0.019	140	0.047±0.12	403	0.21±0.25	485	240±260.6
120002C	191	0.025±0.021	45	0.031±0.02	165	0.31±0.35	197	226±147.5
120301B	290	0.057±0.034	135	0.03±0.019	263	0.2±0.21	458	165±76.99
120302B	317	0.011±0.018	101	0.04±0.036	290	0.15±0.2	401	105.3±76.64
120310A	120	0.034±0.023	63	0.038±0.037	110	0.16±0.095	173	225.6±215.5
124001B	60	0.018±0.013	24	0.016±0.0062	43	0.069±0.061	60	272.5±259.8
1240062	137	0.031±0.021	62	0.033±0.017	127	0.13±0.11	106	2170±7031
125013A	708	0.038±0.023	202	0.033±0.029	649	0.13±0.16	733	154.7±74.85
126001A	405	0.12±0.082	279	0.04±0.022	382	0.13±0.13	426	290.5±211.6

1300000	294	0.1±0.052	100	0.044±0.029	275	0.21±0.16	235	209.5±121.1
130206A	87	0.096±0.047	51	0.037±0.027	88	0.37±0.39	102	352.5±181.1
130302A	150	0.17±0.1	72	0.039±0.026	123	0.33±0.17	166	235.5±126
130504B	114	0.16±0.083	59	0.041±0.044	114	0.59±0.58	113	217.8±144.2
136002D	291	0.035±0.028	150	0.037±0.023	264	0.49±0.87	301	539.7±370.9
136004A	184	0.03±0.016	102	0.023±0.014	183	0.25±0.2	183	255.3±150
136014A	413	0.03±0.028	119	0.036±0.03	358	0.12±0.15	252	398.2±195.9
136094A	67	0.018±0.02	35	0.021±0.01	59	0.11±0.097	57	531.5±618.8
136106A	198	0.049±0.045	119	0.039±0.024	167	0.12±0.069	193	322.1±190.6
138014A	227	0.019±0.017	41	0.026±0.0067	207	0.16±0.11	253	331.1±176.6

Table S-3. Number of samples per water year for each site (water year starts from 1st July to 30th June next year; number indicates the maximum number of samples among all constituents)

Site ID	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016
105107A	36	55	30	39	15	15	38	7	6	25	44
110001D	22	100	102	58	52	83	43	27	86	53	24
110002A	13	29	20	9	0	0	0	0	0	0	0
110003A	15	117	171	82	0	0	0	0	0	0	0
1110056	0	0	0	0	0	0	0	0	84	134	59
1111019	0	0	0	0	0	0	0	0	91	124	109
1120049	0	0	0	0	0	0	45	31	19	47	44
112004A	3	36	26	6	67	4	3	8	16	0	0
112101B	1	57	78	100	75	10	20	54	35	43	43
113006A	12	26	55	136	266	133	266	157	132	158	130
113015A	0	0	0	0	206	28	27	32	79	55	38
116001F	0	0	0	0	107	58	73	56	67	44	53
119101A	0	0	0	0	196	158	184	47	79	104	112
120001A	35	27	46	44	127	48	65	27	28	18	26
120002C	6	16	10	24	24	30	27	11	24	15	21
120301B	0	10	17	5	283	79	76	11	0	0	0
120302B	5	20	16	18	171	71	102	3	0	0	0
120310A	0	9	22	5	89	25	26	18	0	0	0
124001B	4	5	31	20	0	0	0	0	0	0	0
1240062	9	0	22	9	0	0	0	1	46	19	35
125013A	11	40	40	28	126	140	159	82	73	22	80
126001A	0	0	0	2	75	57	33	23	49	76	112
1300000	0	8	0	18	107	19	34	20	36	49	37
130206A	0	0	8	6	14	9	20	5	5	19	22
130302A	0	0	0	0	48	2	0	28	28	38	35
130504B	0	11	8	8	27	20	11	8	0	21	17
136002D	11	26	15	9	126	9	11	19	0	37	42
136004A	0	0	14	20	140	4	5	2	0	0	0
136014A	11	12	14	8	85	135	71	108	22	31	17
136094A	11	12	13	3	17	5	6	4	0	0	0
136106A	3	0	9	5	143	9	23	7	0	0	0
138014A	0	0	0	0	0	0	0	7	85	123	38

Table S-4. Summary of statistics of different catchment characteristics at 32 sites

Catchment characteristics		Min	Percentiles					Max
			5th	25th	50th	75th	95th	
Land use	Conservation (%)	0.2	1.0	3.4	10.3	36.1	83.5	95.6
	Dryland agriculture (%)	0.0	0.0	0.3	0.9	2.9	10.3	14.3
	Irrigated agriculture (%)	0.0	0.0	0.0	0.9	1.6	6.5	8.9
	Intensive uses (%)	0.0	0.0	0.1	0.4	1.4	14.7	28.0
	Water (%)	0.1	0.1	0.4	0.6	1.5	3.5	5.2
	Grazing (%)	1.2	4.6	38.0	61.2	79.9	95.4	96.1
	Sugar cane (%)	0.0	0.0	0.0	0.3	6.8	19.7	47.0
Topography	Slope (°)	0.6	0.8	2.0	3.7	5.9	8.0	11.8
	Stream density (km/km^2)	0.4	0.5	0.6	0.9	1.0	1.1	1.1
	Mean elevation (m)	74.3	105.9	270.3	340.0	479.2	720.2	813.5
Soil and	Soil erodibility	0.035	0.035	0.045	0.048	0.052	0.066	0.074
	Mean TN (mg/kg)	0.053	0.062	0.099	0.136	0.254	0.331	0.337
	Clay (%)	17.2	19.2	27.5	30.1	40.6	48.4	52.2
Climate and hydrology	Annual rainfall (mm)	543.4	554.6	683.9	1139.3	1556.4	3023.7	3744.7
	Annual temperature (°C)	18.9	19.0	19.9	21.1	21.9	23.2	23.9
	Annual runoff (ML)	18557.4	93172.7	181157.3	461104.5	1099688.0	3432006.9	7045249.0

Table S-5. The Australian Land Use and Management (ALUM) code and corresponding description of different land use

Land use	Description	ALUM code
Conservation	Land used primarily for conservation purposes, based on maintaining the essentially natural ecosystems present, including: nature conservation, managed resource protection.	111~ 117, 120~125, 130~134
Dryland agriculture	Land used mainly for primary production based on dryland cropping farming systems (excluding grazing and sugar cane). Including: planation forest, perennial horticulture (dryland), seasonal horticulture, land in transition (dryland).	311~314, 331~334, 340~346, 350, 360~365
Irrigated agriculture	Land used mostly for primary production based on irrigated cropping farming (excluding grazing and sugar cane). Including: irrigated plantation forests, irrigated cropping, irrigated perennial horticulture, irrigated seasonal horticulture, and land in transition (irrigated).	410, 411, 430~434, 436, 440~449, 450~454, 460~465.
Intensive uses	Land subject to extensive modification, generally in association with closer residential settlement, commercial or industrial uses. Including manufacturing and industrial, residential and farm infrastructure, utilities, transport and communication, mining, waste treatment and disposal.	530~538, 540~545, 550~555, 560~567, 570~575, 580~584, 590~595.
Water	Lake, reservoir/dam, river, channel, marsh/wetland.	610~614, 620~623, 630~633, 640~643.
Grazing	Grazing native vegetation, grazing modified pastures (Native/exotic pasture mosaic, Woody fodder plants), Grazing irrigated modified pastures.	210, 320, 321, 322, 420
Sugar cane	Dryland Cropping (sugar), Irrigated cropping (sugar).	335, 435

Table S-6. Kurtosis and skewness of 9 variables before and after Box-Cox transformation

		TSS	PN	NO_X	NH_4	DON	FRP	DOP	PP	EC
Kurtosis	Raw data	4.29	3.95	12.22	4.26	1.79	5.01	2.44	5.89	22.06
	Box-Cox	1.95	2.09	3.62	2.10	1.80	2.16	2.39	2.54	2.99
Skewness	Raw data	1.51	1.13	2.88	1.29	0.08	1.72	-0.30	1.75	4.23
	Box-Cox	0.06	0.03	0.00	0.04	-0.15	0.02	-0.09	0.01	0.00

Table S-7. Kurtosis and skewness of 16 catchment characteristics variables before and after log-sinh transformation

Catchment characteristics	Kurtosis		Skewness		One-sample Kolmogorov-Smirnov test p-value
	Raw data	Log-sinh transformed	Raw data	Log-sinh transformed	
Conservation (%)	3.06	2.20	1.19	-0.05	0.90
Dryland agriculture (%)	6.96	2.23	2.13	0.00	0.72
Irrigated agriculture (%)	7.69	3.36	2.23	0.94	0.35
Intensive uses (%)	9.25	4.14	2.54	1.50	0.05
Water (%)	5.40	2.27	1.72	0.03	0.96
Grazing (%)	2.13	2.11	-0.55	-0.54	0.25
Sugar cane (%)	14.27	2.15	3.18	0.66	0.04
Slope (°)	3.41	2.30	0.88	-0.05	0.84
Stream density (km/km2)	2.07	2.09	-0.05	-0.07	0.46
Mean elevation (m)	2.94	2.92	0.67	0.00	0.44
Soil erodibility	3.18	2.60	0.66	0.01	0.46
Mean TN (mg/kg)	1.97	1.92	0.61	0.00	0.72
Clay (%)	2.45	2.72	0.47	0.00	0.42
Annual rainfall (mm)	3.18	1.63	1.12	0.15	0.17
Annual temperature (°C)	2.26	2.26	-0.02	-0.02	0.84
Annual runoff (ML)	10.79	2.74	2.66	0.00	0.99

Note. One-sample Kolmogorov-Smirnov test p-value is computed based on normalised and standardised log-sinh data set, and p-value > 0.01 indicates the acceptance of the null hypothesis that data comes from a standard normal distribution at the 1% significant level.

Table S-8. Cross correlation (Spearman's rank) matrix of catchment characteristics (colour scheme indicates the magnitude of correlation: dark red – strong positive correlation; dark blue – strong negative correlation)

	Conservation	Dryland agriculture	Irrigated agriculture	Intensive uses	Water	Grazing	Sugar cane	Slope	Stream density	Mean elevation	Soil erodibility	Mean TN	Clay	Annual rainfall	Annual temperature	Annual runoff
Conservation	-	-0.42*	0.28	0.58**	0.66**	-0.82**	0.37*	0.87**	0.78**	0.46**	-0.57**	0.78**	0.17	0.83**	0.01	0.60**
Dryland agriculture	-0.42*	-	0.21	0.09	-0.49**	0.34	-0.37*	-0.37	-0.52**	-0.06	0.21	-0.12	0.38*	-0.47**	-0.50**	-0.22
Irrigated agriculture	0.28	0.21	-	0.62**	0.09	-0.29	0.29	0.22	0.35*	0.36*	-0.47**	0.47**	0.39*	0.35*	-0.34	0.14
Intensive uses	0.58**	0.09	0.62**	-	0.48**	-0.59**	0.35	0.52**	0.51**	0.61**	-0.65**	0.80**	0.40*	0.57**	-0.58**	0.37*
Water	0.66**	-0.49**	0.09	0.48**	-	-0.64**	0.60**	0.61**	0.60**	0.31	-0.31	0.49**	-0.15	0.62**	0.13	0.46**
Grazing	-0.82**	0.34	-0.29	-0.59**	-0.64**	-	-0.60**	-0.89**	-0.77**	-0.25	0.43*	-0.81**	-0.33	-0.89**	0.07	-0.28
Sugar cane	0.37*	-0.37*	0.29	0.35	0.60**	-0.60**	-	0.62**	0.62**	-0.07	-0.26	0.52**	-0.02	0.71**	0.16	0.15
Slope	0.87**	-0.37*	0.22	0.52**	0.61**	-0.89**	0.62**	-	0.77**	0.21	-0.51**	0.87**	0.19	0.93**	-0.06	0.38*
Stream density	0.78**	-0.52**	0.35*	0.51**	0.60**	-0.77**	0.62**	0.77**	-	0.39*	-0.58**	0.73**	0.14	0.88**	0.18	0.37*
Mean elevation	0.46**	-0.06	0.36*	0.61**	0.31	-0.25	-0.07	0.21	0.39*	-	-0.58**	0.47**	0.23	0.25	-0.39*	0.28
Soil erodibility	-0.57**	0.21	-0.47**	-0.65**	-0.31	0.43*	-0.26	-0.51**	-0.58**	-0.58**	-	-0.67**	-0.13	-0.60**	0.19	-0.30
Mean TN	0.78**	-0.12	0.47**	0.80**	0.49**	-0.81**	0.52**	0.87**	0.73**	0.47**	-0.67**	-	0.44*	0.87**	-0.37*	0.28
Clay	0.17	0.38*	0.39*	0.40*	-0.15	-0.33	-0.02	0.19	0.14	0.23	-0.13	0.44*	-	0.22	-0.27	-0.15
Annual rainfall	0.83**	-0.47**	0.35*	0.57**	0.62**	-0.89**	0.71**	0.93**	0.88**	0.25	-0.60**	0.87**	0.22	-	0.00	0.35
Annual temperature	0.01	-0.50**	-0.34*	-0.58**	0.13	0.07	0.16	-0.06	0.18	-0.39*	0.19	-0.37*	-0.27	0.00	-	0.06
Annual runoff	0.60**	-0.22	0.14	0.37*	0.46**	-0.28	0.15	0.38*	0.37*	0.28	-0.30	0.28	-0.15	0.35	0.06	-

Note. * $p < 0.05$.
** $p < 0.01$.

Table S-9. Spearman's rank correlation matrix of mean concentration and hydrometric data, proportion of land use and catchment characteristics (colour scheme indicates the magnitude of correlation: dark red – strong positive correlation; dark blue – strong negative correlation).

	TSS	PN	NO_X	NH_4	DON	FRP	DOP	PP	EC
Conservation	-0.71**	-0.64**	0.17	-0.42*	-0.86**	-0.76**	-0.36*	-0.53**	-0.53**
Dryland agriculture	0.47**	0.30*	-0.10	0.21	0.45**	0.42	0.08	0.43	0.39*
Irrigated agriculture	-0.26	-0.19	0.24	-0.03	-0.13	-0.20	-0.15	-0.13	-0.24
Intensive uses	-0.40*	-0.34	0.25	-0.10	-0.45*	-0.47**	-0.44*	-0.20	-0.24
Water	-0.47**	-0.41*	0.26	-0.16	-0.57**	-0.48**	-0.08	-0.46**	-0.30
Grazing	0.70**	0.57**	-0.41*	0.13	0.60**	0.56**	0.41*	0.54**	0.33
Sugar cane	-0.47**	-0.39	0.58**	0.27	-0.24	-0.22	-0.23	-0.46**	0.01
Slope	-0.74**	-0.65**	0.34	-0.13	-0.67**	-0.62**	-0.45*	-0.61**	-0.23
Stream density	-0.70**	-0.57**	0.42*	-0.34	-0.74**	-0.71**	-0.43*	-0.57**	-0.49**
Mean elevation	-0.20	-0.15	-0.11	-0.47**	-0.52**	-0.47**	-0.33	-0.03	-0.54**
Soil erodibility	0.53**	0.42*	0.16	0.34	0.58**	0.75**	0.57**	0.39*	0.25
Mean TN	-0.61**	-0.50**	0.31	-0.16	-0.61**	-0.57**	-0.57**	-0.39*	-0.27
Clay	-0.16	-0.13	0.32	-0.13	-0.14	0.03	-0.02	0.13	-0.08
Annual rainfall	-0.79**	-0.66**	0.38*	-0.15	-0.66**	-0.64**	-0.45**	-0.62**	-0.32
Annual temperature	-0.10	-0.11	0.02	-0.30	-0.20	-0.11	0.27	-0.21	-0.12
Annual runoff	-0.34	-0.44*	-0.02	-0.39*	-0.65**	-0.53**	-0.06	-0.29	-0.27

Note. * $p < 0.05$.
** $p < 0.01$.

Table S-10. Average water quality VFs scores for Cluster one and Cluster two sites

	'Particulate constituents' VF1	'Dissolved nitrogen' VF2	'NOx' VF3	'Dissolved phosphorus' VF4
Cluster one sites	-0.96	-0.84	0.11	-0.02
Cluster two sites	0.44	0.38	-0.05	0.01

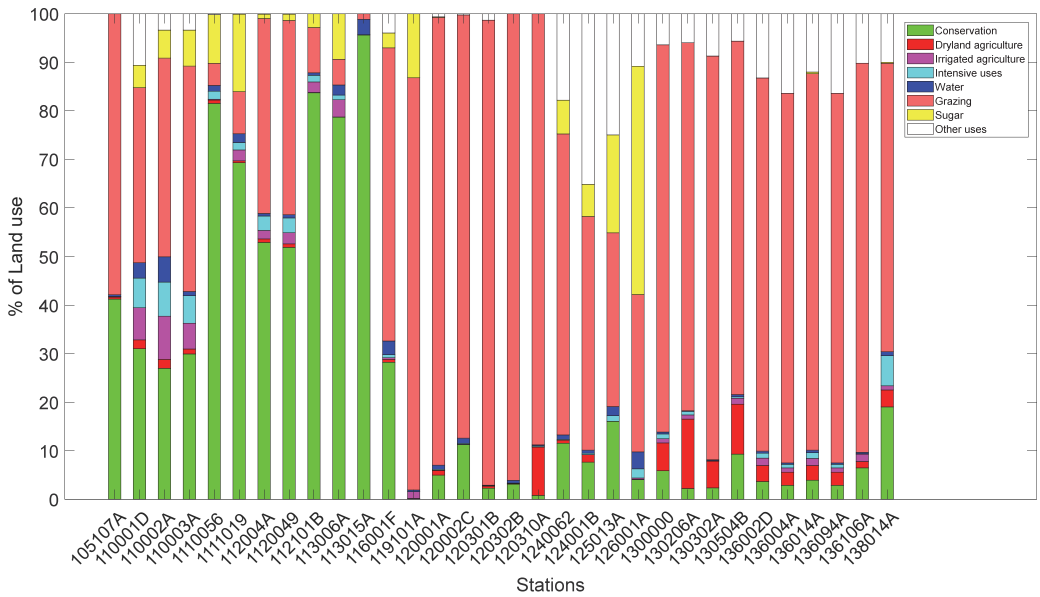

Figure S-1. Land use distribution in 32 sites

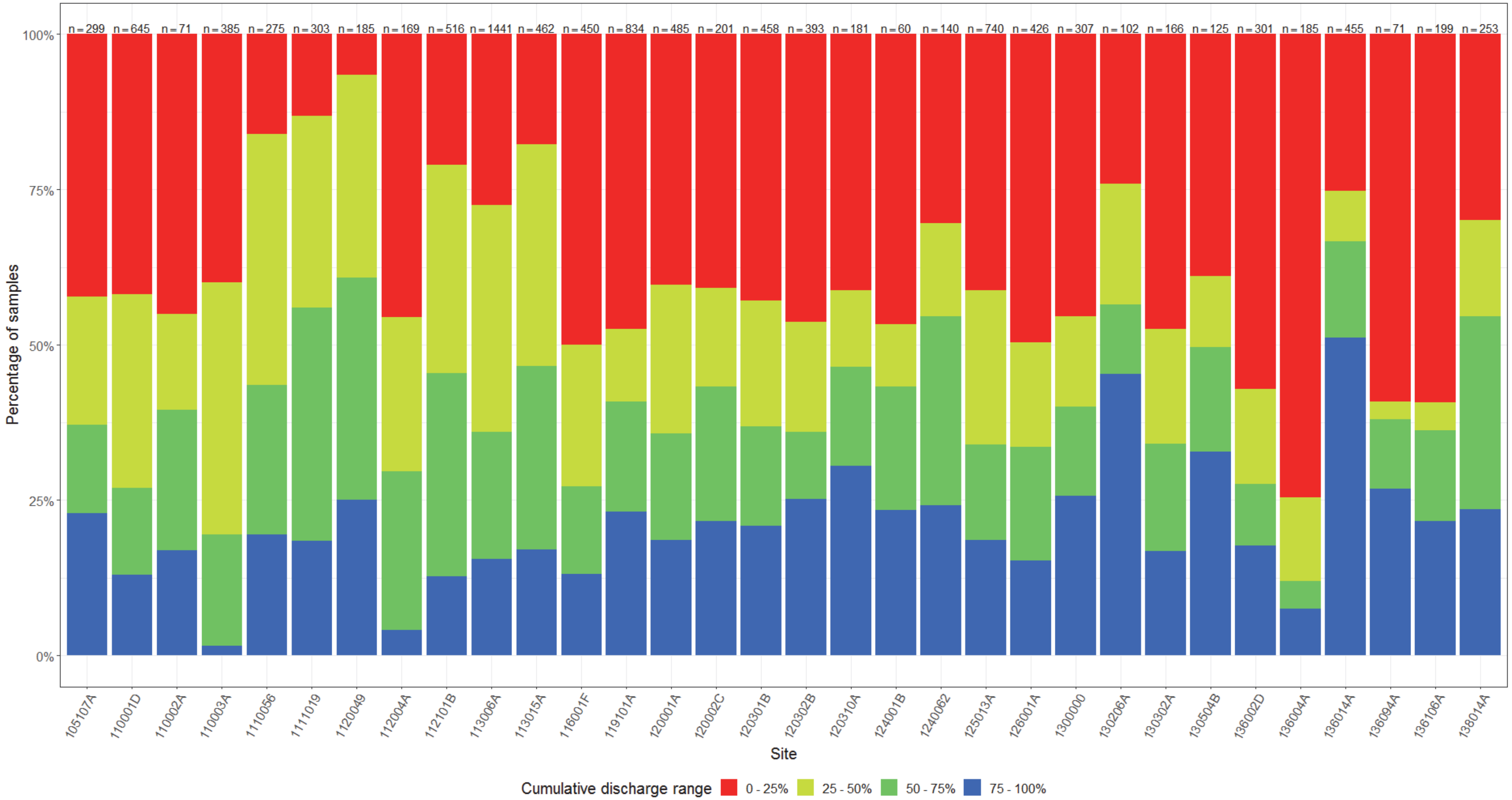

Figure S-2. Percentage of samples falling into the certain range of cumulative discharges for an individual site. The total number of samples is indicated on the top of each stacked bar.

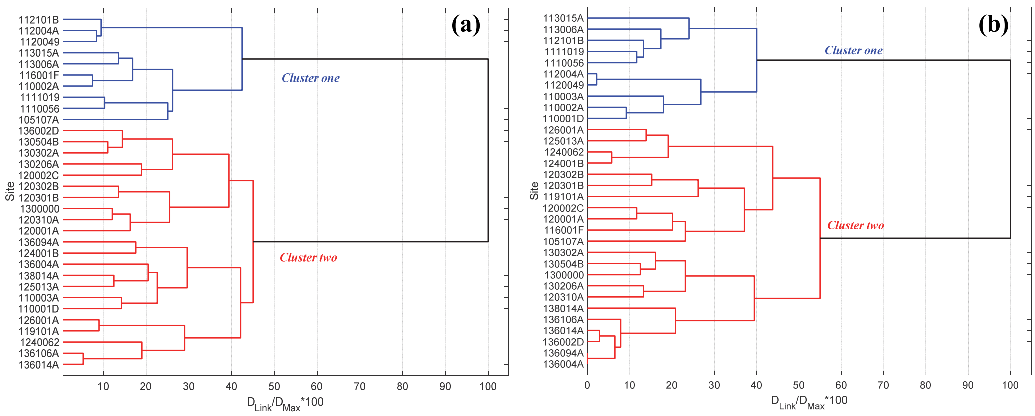

Figure S-3. Results of cluster analysis: (a) Dendrogram illustrates clustering of sites according to surface water quality, and (b) Dendrogram illustrates clustering of sites according to catchment characteristics. Clustering of sites was based on the statistically significant criteria $(D_{Link} / D_{Max}) \times 100 < 60$.

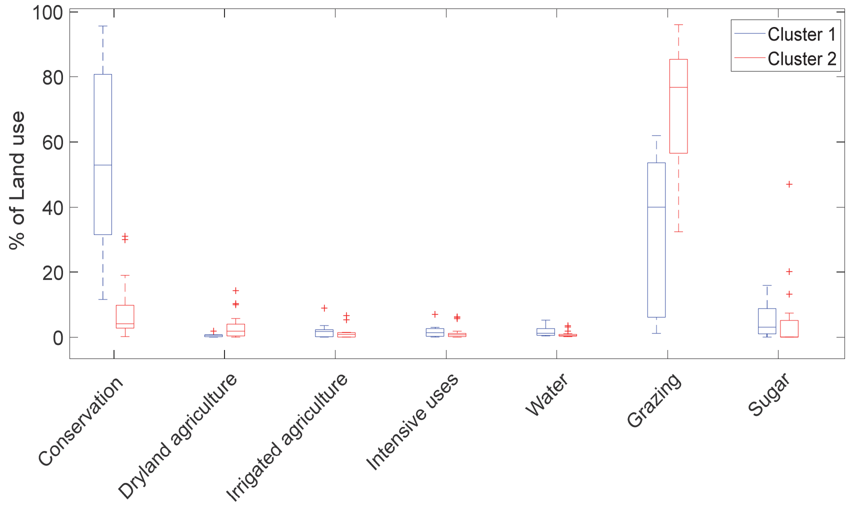

Figure S-4. Comparisons between the two clusters on land use proportions. The horizontal bars from the top to bottom indicate upper whisker, upper quartile, median, lower quartile and lower whisker, respectively. The plus mark indicates the outliers.

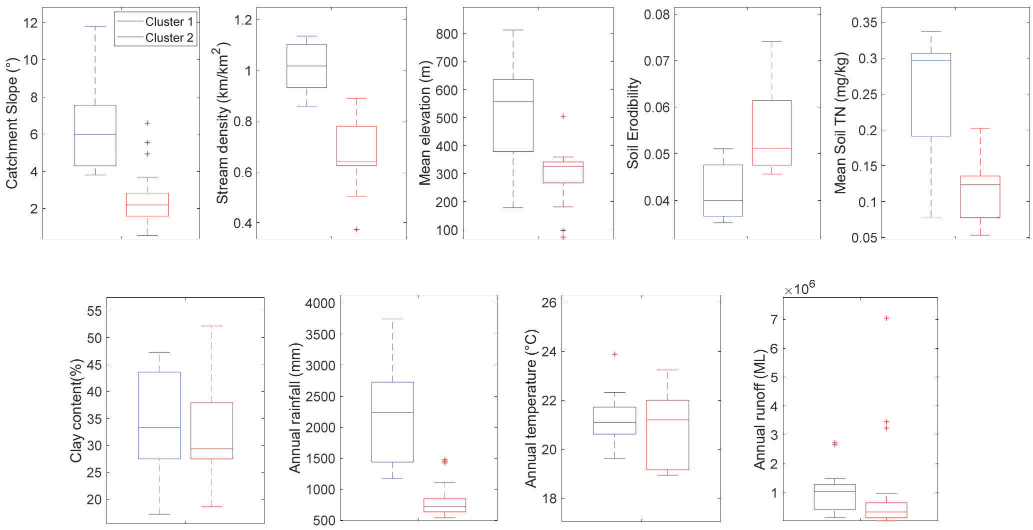

Figure S-5. Comparisons between the two clusters on other catchment characteristics. The horizontal bars from the top to bottom indicate upper whisker, upper quartile, median, lower quartile and lower whisker, respectively. The plus mark indicates the outliers.

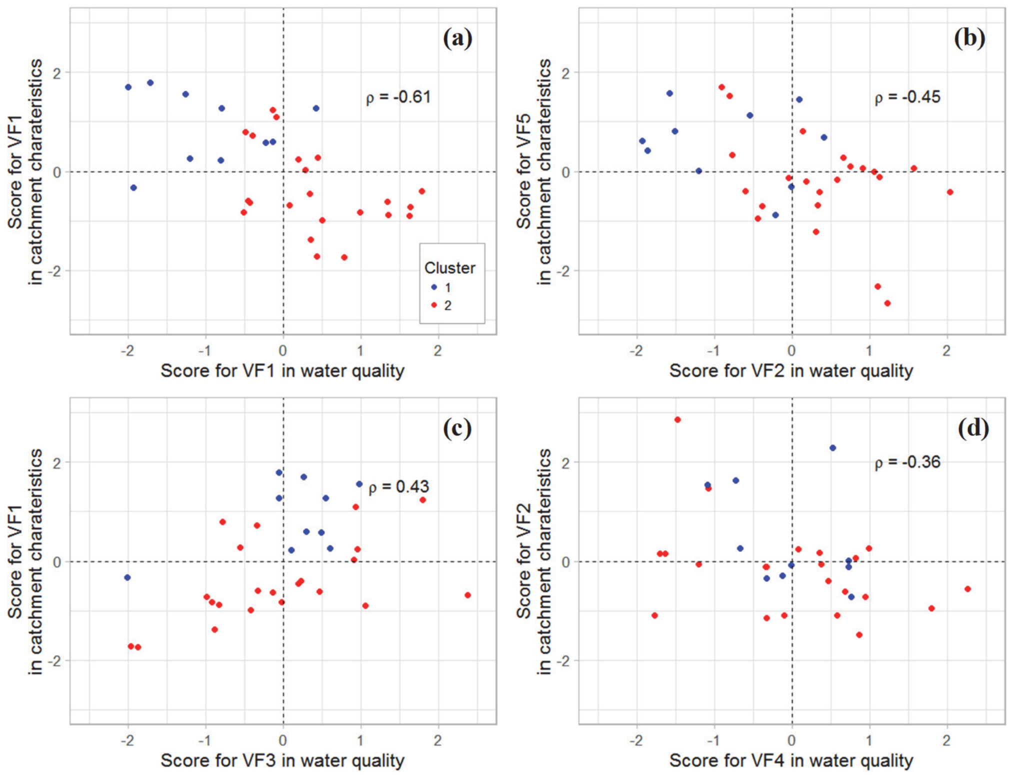

Figure S-6. Scatter plots of relationships between scores for VFs from the water quality PCA/FA and scores for VFs from the catchment characteristics PCA/FA; (a) VF1 in water quality and VF1 in catchment characteristics; (b) VF2 in water quality and VF5 in catchment characteristics; (c) VF3 in water quality and VF1 in catchment characteristics; (d) VF4 in water quality and VF1 in catchment characteristics. Different colours indicate sites in two clusters: blue = Cluster one and red = Cluster two. ρ indicates the Spearman's rank correlation coefficient.

A2. Supplementary Materials for Chapter 5

Table S-11. Summary statistics of site-level mean EMC of nine studied constituents

Constituent	Min	Percentiles					Max
		10^{th}	25^{th}	50^{th}	75^{th}	90^{th}	
TSS (mg/L)	16.42	38.20	73.97	133.65	200.44	530.11	630.20
PN (mg/L)	0.11	0.19	0.36	0.44	0.56	0.79	0.85
NO_X (mg/L)	0.02	0.03	0.07	0.13	0.16	0.24	0.29
NH_4 (mg/L)	0.01	0.01	0.01	0.02	0.03	0.04	0.05
DON (mg/L)	0.10	0.13	0.23	0.35	0.44	0.52	0.59
FRP (mg/L)	0.00	0.01	0.01	0.03	0.04	0.10	0.22
DOP (mg/L)	0.01	0.02	0.02	0.03	0.03	0.04	0.04
PP (mg/L)	0.03	0.06	0.10	0.14	0.21	0.30	0.55
EC (µS/cm)	28.57	41.55	84.95	205.31	274.29	543.57	5180.01

Table S-12. Shapiro-Wilk's test p-value of site-level average EMCs before and after Box Cox transformation

Constituent	Shapiro-Wilk's test p-value	
	Raw data	Box Cox transformed
TSS	0.000	0.620
PN	0.135	0.228
NO_X	0.285	0.582
NH_4	0.003	0.388
DON	0.114	0.094
FRP	0.000	0.598
DOP	0.743	0.777
PP	0.002	0.935
EC	0.000	0.371

Note: Shapiro-Wilk's test p-value is computed to test the normality before and after Box-Cox transformation of site-level mean EMCs. A p-value > 0.01 indicates the acceptance of the null hypothesis that data comes from a normal distribution at the 1% significant level.

Table S-13. Description and source of 58 catchment characteristics

Catchment characteristic		Abbreviation used in figures and tables in paper	Averaging method and time span	Source
Topography	Maximum catchment elevation (m)	Max_Elevation	Areal average of gridded data; 1976-2005	Geoscience Australia (2011)
	Mean catchment elevation (m)	Mean_Elevation		
	Catchment area (km^2)	Area		
	Stream density (km/km^2)	StreamDensity		
	catchment relief ratio	CatRelifRatio		

	Area of catchment made up of valley bottoms (%)	Valley_Bottoms		
	Mean catchment slope (%)	MeanCatSlope		
	Total catchment length (km)	CatLength		
	Mean channel slope (%)	ChannelSlope		
Land cover	% catchment covered with grasses: grasslands with tussock, hummock, reeds/rushes	Grasses	Areal average of gridded data; 1976-2005	Geoscience Australia (2011)
	% catchment covered with forest: to rainforests, Eucalypt forests, mangroves and low closed forests (e.g., Acacia, Melaleuca or Banksia species). Areas with high density of vegetation (>30% cover) and tall trees (>10 m).	Forest		
	% catchment covered with shrubs: open and dry woodlands and shrublands with hummock or tussock grass, Melaleuca shrublands, lignum shrublands, saltbush and chenopods. Areas with vegetation <2 m tall	Shrubs		
	% catchment covered with woodland: areas with medium trees (<10 m) at medium density (<30% cover).	Woodland		
	% catchment that is bare.	Bare		
	Average width of vegetated riparian zone	MeanVegW_m	Areal average of gridded data; 2013	Queensland Government (2017); Clark et al., (2015). Riparian vegetation is measured using Landsat 5 Thematic Mapper (TM), Landsat 7 Enhanced Thematic Mapper (ETM+) and Landsat 8 Operational Land Imager (OLI) satellite imagery.
	Average catchment riparian zone fragmentation	FraRipaZone		
Land use	Land used primarily for conservation purposes, based on maintaining the essentially natural ecosystems present, such as national park.	PerConservation	Areal average of polygons; 2013	Queensland Government (2017)

	Land used mainly for primary production based on dryland farming systems (excluding grazing and sugar cane).	PerDrylandAgri		
	Land used mostly for primary production based on irrigated farming (excluding grazing and sugar cane).	PerIrrigated		
	Lake, reservoir/dam, river, channel, marsh/wetland.	PerWater		
	Grazing native vegetation, Grazing modified pastures (Native/exotic pasture mosaic, Woody fodder plants), Grazing irrigated modified pastures.	PerGrazing		
	Dryland sugar and Irrigated sugar.	PerSugar		
	Land subject to extensive modification, generally in association with closer residential settlement, commercial or industrial uses (e.g. urban, utilities, roads).	PerIntensiveUses		
	% Catchment used for cropping: the production of commodities such as cereals, beverage and spice crops, hay, oilseeds, sugar, cotton, alkaloid poppies and pulses	PerCropping	Areal average of gridded data; 2010-2011	Geoscience Australia (2011)
	% Catchment with perennial & seasonal horticulture	PerHorti		
	% Catchment fertilized	PerFertilized		
	% Catchment used for forestry	PerForestry		
	% Catchment urbanized	PerUrbanized		
	Maximum barrier free flow path length upstream (reservoirs) (km)	UpstreamReser		
	Maximum barrier free flow path length upstream (damwalls) (km)	UpstreamDam		
Geology	% catchment underlain by regolith - unconsolidated materials (e.g. colluvium and alluvial)	PerUnconsolidated	Areal average of gridded data	Geoscience Australia (2011)
	% catchment underlain by igneous rock	PerIgneous		
	% mixed igneous and sedimentary	PerMixIgSed		
	% catchment underlain by certain types of sedimentary rock	PerSedimentary		
	Cation exchange capacity (mean) of the soil within the 0 - 5 cm depth layer in catchment	MeanCaExCap		
	% area of catchment classed as acid sulfate level B	PerAcidS_B		
	Mean TN levels in soil in catchment (natural condition) (mg/kg)	MeanTN	Areal average of gridded data; 1950-2013	Terrestrial Ecosystem Research Network (2016)
	Mean TP levels in soil in catchment (natural condition) (mg/kg)	MeanTP		
	0-30cm Clay Content (%)	Clay_30		
	Mean soil erodibility in catchment	MeanSoilEro		

	0-30cm pH	pH	Areal average of gridded data; 2011	ASRIS (2011)
	0-1m Plant Available Water Capacity (mm)	PAWC		
	0-30cm Bulk Density (mg/m3)	Bulk_density		
Climate	Average annual radiation (MJ/m2/day)	AnnRad	Areal average of gridded data; 1976-2005	Geoscience Australia (2011)
	Average temperature (degrees Celsius)	AnnTemp		
	Minimum temperature of coldest month (degrees Celsius)	ColdMonthTemp		
	Maximum temperature of hottest month (degrees Celsius)	HotMonthTemp		
	Annual average rainfall (mm)	AnnRain		
	Average rainfall of the warmest quarter (mm)	WarmQRain		
	Average rainfall of the coldest quarter (mm)	ColdQRain		
	Annual average catchment rainfall erosivity (MJ mm/ha hr yr)	Erosivity		
Hydrology	Average annual runoff (mm)	AnnRun	Areal average of gridded data; 1970-2008	Geoscience Australia (2011)
	Maximum annual runoff (mm)	MaxRun		
	Pereniality of runoff (%) - % contribution to mean annual discharge by the six driest months of the year	RunPereniality		
	Mean Base Flow Index	Mean_BFI	Point data; 2006 to 2016	Calculated based on annual average BFI
	Runoff ratio	Mean_RR		Calculated using instantaneous flows from DNRME (2018) and daily catchment rainfall from Australian Water Availability Project (AWAP)- annual average RR from 2006 to 2016
	Mean number of days where there is no flow annually (days/year)	Cease_to_Flow		Calculated using instantaneous flows from DNRME (2018)
	Mean 7-day low flow (ML/d)	Sevendaylowflow		

Table S-14. Summary statistics of 58 catchment characteristics

Catchment characteristics		Min	Percentiles					Max
			10th	25th	50th	75th	90th	
Topography	Maximum catchment elevation (m)	599	859	958	1153	1262	1338	1617
	Mean catchment elevation (m)	74	185	270	340	466	608	813
	Catchment area (km2)	240	409	835	6999	17806	35188	139163
	Stream density (km/km2)	0.37	0.62	0.63	0.85	0.97	1.09	1.13
	catchment relif ratio	0.00	0.00	0.00	0.00	0.01	0.02	0.03
	Area of catchment made up of valley bottoms (%)	0.42	1.76	5.10	7.42	20.72	33.65	40.70
	Mean catchment slope (%)	0.55	1.38	2.01	3.74	5.89	7.52	11.80
	Total catchment length (km)	49.72	70.84	119.95	336.09	531.39	882.79	1060.23
	Mean channel slope (%)	0.00	0.01	0.01	0.02	0.04	0.05	0.10
Land cover	% catchment covered with grasses (present)	0.00	0.00	0.01	0.33	1.00	1.61	6.23
	% catchment covered with forest (present)	0.01	1.33	9.27	16.46	41.36	73.34	88.59
	% catchment covered with shrubs (present)	0.00	0.00	0.00	0.32	1.00	4.56	6.35
	% catchment covered with woodland (present)	0.71	2.22	14.73	31.47	46.22	72.08	93.36
	% catchment that is bare (present)	0.00	0.00	0.00	0.00	0.00	0.00	0.31
	Average width of vegetated riparian zone	105.66	154.01	160.01	186.75	202.95	208.70	220.66
	Average catchment riparian zone fragmentation	48.38	64.40	71.41	79.78	89.38	95.41	97.65
Land use	Area of catchment used for conservation (%)	0.15	2.30	3.54	10.32	33.58	77.77	95.65
	Area of catchment used for dryland agriculture (%)	0.00	0.03	0.32	0.85	2.77	5.72	14.30

	Area of catchment used for irrigated agriculture (%)	0.00	0.01	0.04	0.88	1.57	3.42	8.90
	Area of catchment used for water (%)	0.12	0.21	0.36	0.60	1.35	3.11	5.22
	Area of catchment used for grazing (%)	1.15	8.73	39.00	61.15	79.81	88.57	96.06
	Dryland Cropping (sugar), Irrigated cropping (sugar).	0.00	0.00	0.00	0.27	6.69	12.89	47.02
	Area of catchment used for intensive (%)	0.00	0.00	0.06	0.43	1.37	12.32	28.01
	Area of catchment used for cropping (%)	0.00	0.08	0.52	2.47	4.54	12.51	39.98
	% Catchment with perennial&seasonal horticulture	0.00	0.00	0.00	0.03	0.36	2.07	3.20
	% Catchment fertilized	0.02	0.51	4.04	8.02	16.39	23.13	48.94
	% Catchment used for forestry	0.00	0.04	0.48	5.64	12.77	17.63	35.03
	% Catchment urbanized	0.00	0.01	0.03	0.09	0.25	0.37	1.97
	Maximum barrier free flow path length upstream (reservoirs) (km)	28.65	39.15	60.23	103.41	214.69	270.43	502.80
	Maximum barrier free flow path length upstream (dam walls) (km)	0.38	32.22	49.95	94.93	189.06	298.90	502.80
Geology	% catchment underlain by regolith	0.00	1.52	7.32	21.91	32.79	52.06	76.86
	% catchment underlain by igneous rock	0.29	9.04	17.20	40.05	73.26	86.57	100.00
	% mixed igneous and sedimentary	0.00	0.00	0.00	0.22	4.38	7.67	42.70
	% catchment underlain by certain types of sedimentary rock	0.00	0.02	1.92	18.22	33.02	51.47	94.32

	Cation exchange capacity (mean) of the soil within the 0 - 5 cm depth layer in catchment	3.42	4.48	5.44	7.42	10.37	11.11	12.34
	Mean TN levels in soil in catchment	0.05	0.07	0.10	0.14	0.25	0.30	0.34
	Mean TP levels in soil in catchment	0.00	0.01	0.02	0.03	0.04	0.07	0.08
	% area of catchment classed as acid sulfate level B	8.35	18.27	27.33	40.84	57.48	78.01	97.19
	Mean soil erodibility in catchment (	0.04	0.04	0.05	0.05	0.05	0.06	0.07
	0-30cm Clay Content (%)	17.23	25.75	27.51	30.08	40.25	46.40	52.20
	0-30cm pH	4.55	4.88	5.27	5.50	5.87	6.33	6.82
	0-1m Plant Available Water Capacity (mm)	39.00	52.12	71.08	79.27	94.46	112.64	168.00
	0-30cm Bulk Density (mg/m3)	1.16	1.35	1.40	1.50	1.52	1.53	1.60
Climate	Average annual radiation (MJ/m2/day)	17.73	18.18	18.62	19.10	19.71	20.48	20.67
	Average temperature (degrees Celsius)	18.94	19.07	20.00	21.15	21.87	22.30	23.88
	Minimum temperature of coldest month (degrees Celsius)	3.66	4.46	5.81	9.87	10.85	12.11	14.75
	Maximum temperature of hottest month (degrees Celsius)	28.53	29.19	29.69	30.91	32.74	33.92	34.88
	Annual average rainfall (mm)	543.44	621.75	689.25	1139.35	1534.79	2719.40	3744.73
	Average rainfall of the warmest quarter (mm)	254.00	287.56	308.42	531.49	813.45	1105.44	1532.84
	Average rainfall of the coldest quarter (mm)	36.19	58.39	82.40	102.39	150.77	328.52	430.63

	Annual average catchment rainfall erosivity (MJ mm/ha hr yr)	2021.33	2051.56	2256.93	5357.99	10083.15	15528.32	26997.00
Hydrology	Average annual runoff (mm)	18557	96480	183384	461105	1081221	2717981	7045249
	Maximum annual runoff (mm)	329582	611972	1328796	2544379	4676861	9122645	66056510
	Pereniality of runoff (%)	0.21	0.69	1.36	4.01	6.47	7.73	11.85
	Mean Base Flow Index	0.10	0.16	0.23	0.33	0.52	0.69	0.73
	Runoff ratio	0.00	0.05	0.06	0.21	0.43	0.77	0.94
	Mean number of days where there is no flow annually (days/year)	0.00	0.00	0.00	0.42	19.30	39.58	46.22
	Mean 7-day low flow (ML/d)	0.00	0.00	0.00	0.01	0.11	0.15	0.18

Table S-15. Shapiro-Wilk's test p-value of catchment characteristics before and after Log-sinh transformation.

Catchment characteristic		Shapiro-Wilk's test p-value	
		Raw data	Log-sinh transformed
Topography	Max_Elevation	0.631	0.666
	Mean_Elevation	0.090	0.549
	Area	0.000	0.030
	StreamDensity	0.145	0.146
	CatRelifRatio	0.001	0.034
	Valley_Bottoms	0.000	0.330
	MeanCatSlope	0.027	0.816
	CatLength	0.001	0.010
	ChannelSlope	0.003	0.943
Land cover	Grasses	0.000	0.020
	Forest	0.000	0.656
	Shrubs	0.000	0.000
	Woodland	0.018	0.035
	Bare	0.000	0.000
	MeanVegW_m	0.028	0.213
	FraRipaZone	0.182	0.413
Land	PerConservation	0.000	0.222

	PerDrylandAgri	0.000	0.292
	PerIrrigated	0.000	0.002
	PerWater	0.000	0.634
	PerGrazing	0.014	0.014
	PerSugar	0.000	0.000
	PerIntensiveUses	0.000	0.000
	PerCropping	0.000	0.000
	PerHorti	0.000	0.001
	PerFertilized	0.000	0.902
	PerForestry	0.001	0.010
	PerUrbanized	0.000	0.530
	UpstreamReser	0.001	0.402
	UpstreamDam	0.001	0.641
Geology	PerUnconsolidated	0.014	0.590
	PerIgneous	0.080	0.289
	PerMixIgSed	0.000	0.000
	PerSedimentary	0.000	0.004
	MeanCaExCap	0.026	0.032
	MeanTN	0.003	0.091
	MeanTP	0.002	0.288
	PerAcidS_B	0.176	0.747
	MeanSoilEro	0.042	0.162
	Clay_30	0.043	0.117
	pH	0.454	0.800
	PAWC	0.051	0.277
	Bulk_density	0.001	0.056
Climate	AnnRad	0.270	0.376
	AnnTemp	0.169	0.170
	ColdMonthTemp	0.050	0.040
	HotMonthTemp	0.026	0.144
	AnnRain	0.000	0.015
	WarmQRain	0.001	0.004
	ColdQRain	0.000	0.204
	Erosivity	0.000	0.003
Hydrology	AnnRun	0.000	0.922
	MaxRun	0.000	0.855
	RunPereniality	0.024	0.082
	Mean_BFI	0.029	0.257
	Mean_RR	0.000	0.128
	Cease_to_Flow	0.000	0.000

Sevendaylowflow	0.000	0.004

Note: Shapiro-Wilk's test p-value is computed to test the normality before and after Log-sinh transformation of catchment characteristics. A p-value > 0.01 indicates the acceptance of the null hypothesis that data comes from a normal distribution at the 1% significant level.

Table S-16. Summary of plausible models for nine constituents. (models with a ΔCAIC < 2 was selected as plausible model, and CAIC model Weight calculated based on ΔCAIC, similar to Equation 5-2 but in a CAIC form)

Model ID	Model predictor and coefficients	CAIC Weight	NSE	No. of predictor
	TSS			
1	-0.407*PerUnconsolidated -0.923*AnnRain	0.115	0.631	2
2	-0.504*PerUnconsolidated -6.511*AnnRain + 0.801*MeanTN + 4.876*WarmQRain + 0.336*RunPereniality	0.104	0.756	5
3	-0.498*PerUnconsolidated -2.213*AnnRain - 0.685*ColdMonthTemp + 1.870*Erosivity	0.089	0.716	4
4	-0.428*PerUnconsolidated -4.691*AnnRain + 0.819*MeanTN + 3.094*WarmQRain	0.088	0.716	4
5	-0.586*PerUnconsolidated -2.531*AnnRain + 1.537*WarmQRain	0.082	0.672	3
6	-0.661*PerUnconsolidated -4.439*AnnRain + 3.393*WarmQRain + 0.343*RunPereniality	0.076	0.713	4
7	-0.548*PerUnconsolidated -3.567*AnnRain - 0.562*ColdMonthTemp + 3.061*WarmQRain	0.076	0.713	4
8	-0.553*PerUnconsolidated -1.735*AnnRain + 0.770*Erosivity	0.061	0.666	3
9	-0.38*PerUnconsolidated -3.16*AnnRain -0.62*AnnTemp + 2.43*Erosivity	0.060	0.709	4
10	-0.403*PerUnconsolidated + 0.341*MeanTP -4.343*AnnRain - 0.578*ColdMonthTemp + 3.726*WarmQRain	0.056	0.746	5
11	0.625*StreamDensity + 0.550*MeanTP -2.320*AnnRain - 1.666*ColdMonthTemp + 2.649*Erosivity -0.657*ColdQRain	0.055	0.779	6
12	0.612*MeanTP -1.639*AnnRain -1.425*ColdMonthTemp + 2.363*Erosivity -0.718*ColdQRain	0.051	0.744	5
13	-0.426*PerUnconsolidated + 0.566*StreamDensity -2.744*AnnRain -0.971*ColdMonthTemp + 2.146*Erosivity	0.047	0.743	5
14	-0.526*PerUnconsolidated + 0.317*MeanTP -5.085*AnnRain + 3.925*WarmQRain + 0.335*RunPereniality	0.043	0.742	5
	PN			
1	-0.533*Area -0.744*PerUnconsolidated -1.278*AnnRain	0.217	0.618	3
2	0.610*CatRelifRatio -0.748*PerUnconsolidated -1.374*AnnRain	0.191	0.614	3
3	-0.623*PerConservation -0.956*PerUnconsolidated + 0.467*HotMonthTemp	0.166	0.611	3
4	-0.593*Area -0.878*PerUnconsolidated -1.052*AnnRain + 0.405*HotMonthTemp	0.094	0.650	4
5	-0.744*PerUnconsolidated -0.909*AnnRain -0.272*MaxRun	0.090	0.596	3

6	-0.665*PerConservation -0.792*PerUnconsolidated + 0.583*HotMonthTemp + 0.344*MeanTP	0.081	0.646	4
7	-0.711*PerUnconsolidated -0.743*AnnRain -0.262*AnnRun	0.081	0.593	3
8	-0.665*PerUnconsolidated -0.797*AnnRain	0.080	0.532	2
	NO_X			
1	-0.595*Mean_Elevation + 1.655*StreamDensity + 1.093*MeanVegW_m + 0.737*PerCropping + 0.679*pH - 1.798*ColdMonthTemp	0.424	0.804	6
2	-0.601*Mean_Elevation + 1.438*StreamDensity + 1.093*MeanVegW_m + 0.723*PerCropping + 0.667*pH - 1.768*ColdMonthTemp -0.245*Cease_to_Flow	0.368	0.828	7
3	-0.584*Mean_Elevation + 1.322*StreamDensity + 1.090*MeanVegW_m + 0.710*PerCropping + 0.834*pH - 1.479*ColdMonthTemp -0.270*Cease_to_Flow + 0.221*RunPereniality	0.207	0.845	8
	NH_4			
1	0.613*Woodland -0.269*Bare + 0.842*PerSugar -0.336*PerHorti - 0.318*PerCropping -1.455*AnnRad -1.439*WarmQRain	0.119	0.856	7
2	0.405*Woodland + 0.516*MeanCatSlope -0.179*Bare + 0.499*PerSugar -0.270*PerHorti -1.660*AnnRad - 2.077*WarmQRain -0.462*RunPereniality	0.092	0.873	8
3	0.392*Woodland + 0.592*MeanCatSlope + 0.517*PerSugar - 0.258*PerHorti -1.854*AnnRad -2.256*WarmQRain - 0.548*RunPereniality	0.088	0.853	7
4	0.479*Woodland -0.846*Mean_Elevation -0.523*StreamDensity - 0.237*Bare + 1.110*PerSugar -0.343*PerHorti -0.539*PerCropping -1.235*AnnTemp + 0.578*PerConservation -0.435*PerForestry	0.082	0.903	10
5	0.428*Woodland + 0.466*ChannelSlope -0.202*Bare + 0.400*PerSugar -0.283*PerHorti -1.760*AnnRad - 2.032*WarmQRain -0.485*RunPereniality	0.075	0.871	8
6	0.700*MeanCatSlope + 0.534*PerSugar -0.254*PerHorti - 1.764*AnnRad -2.542*WarmQRain -0.781*RunPereniality	0.068	0.828	6
7	1.038*Woodland -1.080*StreamDensity -0.303*Bare + 1.016*PerSugar -0.381*PerHorti -0.476*PerCropping - 1.372*AnnRad -0.591*AnnTemp -0.494*PerForestry	0.065	0.887	9
8	-0.754*Mean_Elevation + 0.304*ChannelSlope -0.249*PerHorti - 1.022*AnnTemp -0.347*RunPereniality	0.064	0.802	5
9	0.962*Woodland -0.695*StreamDensity -0.308*Bare + 1.094*PerSugar -0.396*PerHorti -0.496*PerCropping - 1.554*AnnRad -0.401*AnnTemp -0.658*WarmQRain - 0.422*PerForestry	0.055	0.900	10
10	0.603*Woodland + 0.491*MeanCatSlope -0.221*Bare + 0.566*PerSugar -0.290*PerHorti -1.207*AnnRad - 1.637*WarmQRain	0.052	0.848	7
11	-0.739*Mean_Elevation + 0.688*ChannelSlope + 0.356*PerSugar - 0.351*PerHorti -1.360*AnnTemp -1.670*WarmQRain + 1.334*ColdMonthTemp	0.051	0.848	7
12	0.361*Woodland -0.639*Mean_Elevation + 0.464*ChannelSlope - 0.262*PerHorti -0.892*AnnTemp	0.050	0.799	5
13	0.858*Woodland -0.247*Mean_Elevation -0.788*StreamDensity - 0.269*Bare + 0.983*PerSugar -0.377*PerHorti -0.505*PerCropping -1.033*AnnRad -0.758*AnnTemp -0.469*PerForestry	0.047	0.899	10
14	0.298*MeanCatSlope -0.760*Mean_Elevation -0.243*PerHorti - 1.012*AnnTemp -0.362*RunPereniality	0.047	0.798	5

15	0.679*Woodland -0.253*Bare + 0.508*PerSugar -0.313*PerHorti - 1.449*AnnRad -1.291*WarmQRain	0.046	0.824	6
	DON			
1	-0.533*Mean_Elevation + 0.571*Area -0.210*PerIgneous - 0.805*AnnTemp -0.539*MaxRun -0.423*RunPereniality	0.126	0.971	6
2	-0.108*Max_Elevation -0.352*CatLength -0.288*Bare - 0.215*PerIgneous -0.235*AnnTemp -0.717*AnnRad - 1.180*AnnRain -0.363*RunPereniality -0.116*AnnRun - 0.334*Mean_RR	0.100	0.983	10
3	-0.239*Area -0.561*CatLength -0.313*Bare -0.203*PerIgneous - 0.800*AnnRad -0.414*RunPereniality -1.769*WarmQRain - 0.349*Mean_RR	0.086	0.978	8
4	-0.100*Max_Elevation -0.348*CatLength -0.273*Bare - 0.225*PerIgneous -0.247*AnnTemp -0.750*AnnRad - 0.120*MaxRun -1.266*AnnRain -0.364*RunPereniality - 0.327*Mean_RR	0.073	0.983	10
5	-0.5066*CatLength -0.2507*Bare -0.2127*PerIgneous + 0.0952*PerForestry -0.7531*AnnRad -0.1351*MaxRun - 0.3979*RunPereniality -1.5993*WarmQRain -0.2280*Mean_RR	0.071	0.980	9
6	-0.0854*Max_Elevation -0.4191*CatLength -0.2548*Bare - 0.1973*PerIgneous + 0.1036*PerForestry -0.7381*AnnRad - 0.1157*MaxRun -0.3844*RunPereniality -1.4373*WarmQRain - 0.2646*Mean_RR	0.066	0.983	10
7	-0.0889*Max_Elevation -0.2126*Area -0.4247*CatLength - 0.2856*Bare -0.2015*PerIgneous + 0.0828*PerForestry - 0.7037*AnnRad -0.3600*RunPereniality -1.5264*WarmQRain - 0.3130*Mean_RR	0.065	0.983	10
8	-0.2457*Area -0.5219*CatLength -0.2871*Bare - 0.2181*PerIgneous + 0.0702*PerForestry -0.7118*AnnRad - 0.3691*RunPereniality -1.7122*WarmQRain -0.2821*Mean_RR	0.058	0.980	9
9	-0.3992*CatLength -0.2281*Bare -0.1931*PerIgneous + 0.0979*PerForestry -0.1031*MeanVegW_m -0.7632*AnnRad - 0.1254*MaxRun -0.4422*RunPereniality -1.4799*WarmQRain - 0.1892*Mean_RR	0.056	0.983	10
10	-0.195*Grasses -0.259*Bare -0.156*PerIgneous -0.900*AnnRad - 0.256*MaxRun -1.312*AnnRain -0.410*RunPereniality - 0.283*Mean_RR	0.054	0.977	8
11	-0.510*Mean_Elevation + 0.421*Area -0.210*PerIgneous - 0.862*AnnTemp -0.473*MaxRun + 0.136*HotMonthTemp - 0.428*RunPereniality	0.053	0.974	7
12	-0.391*CatLength -0.265*Bare -0.229*PerIgneous - 0.226*AnnTemp -0.833*AnnRad -0.153*MaxRun -1.475*AnnRain -0.386*RunPereniality -0.279*Mean_RR	0.052	0.980	9
13	-0.0957*Max_Elevation -0.4235*CatLength -0.2727*Bare - 0.1872*PerIgneous + 0.0989*PerForestry -0.7039*AnnRad - 0.3779*RunPereniality -1.3482*WarmQRain -0.1062*AnnRun - 0.2759*Mean_RR	0.048	0.982	10
14	-0.495*CatLength -0.105*Grasses -0.285*Bare -0.194*PerIgneous - 0.656*AnnRad -0.145*MaxRun -0.374*RunPereniality - 1.498*WarmQRain -0.289*Mean_RR	0.048	0.980	9
15	-0.361*CatLength -0.187*Bare -0.218*PerIgneous + 0.127*PerForestry -0.129*MeanVegW_m -0.751*AnnRad - 0.121*MaxRun -0.451*RunPereniality -1.562*WarmQRain	0.047	0.980	9
	FRP			
1	-0.864*Valley_Bottoms -0.173*Bare -0.366*MeanVegW_m + 0.798*PerSugar + 0.145*PerHorti + 0.199*PerMixIgSed -	0.668	0.950	10

	0.539*PerAcidS_B + 0.693*pH + 0.816*AnnTemp - 1.114*ColdMonthTemp			
2	-0.940*Valley_Bottoms -0.264*Bare -0.487*FraRipaZone + 0.737*PerSugar + 0.139*PerHorti + 0.192*PerMixIgSed - 0.619*PerAcidS_B + 0.483*pH + 0.946*AnnTemp - 1.246*ColdMonthTemp	0.332	0.948	10
	DOP			
1	0.605*Grasses -0.939*Shrubs -0.640*PerIntensiveUses + 0.294*PerMixIgSed -0.834*Erosivity	0.163	0.674	5
2	0.759*Grasses -0.813*Shrubs -0.762*PerIntensiveUses + 0.339*PerMixIgSed -2.697*Erosivity + 2.020*WarmQRain	0.123	0.711	6
3	0.476*Grasses -0.873*Shrubs -0.619*PerIntensiveUses + 0.281*PerCropping -0.903*Erosivity	0.111	0.666	5
4	-0.437*MeanCatSlope -0.663*PerIntensiveUses + 0.507*PerFertilized	0.097	0.555	3
5	0.785*Valley_Bottoms -0.638*PerIntensiveUses + 0.619*PerFertilized -0.372*PerUrbanized - 0.666*PerUnconsolidated	0.094	0.663	5
6	-0.623*MeanCatSlope -0.381*Shrubs -0.708*PerIntensiveUses + 0.371*PerFertilized	0.092	0.611	4
7	-0.673*Shrubs + 1.073*HotMonthTemp	0.090	0.486	2
8	0.788*Valley_Bottoms -0.726*PerIntensiveUses + 0.415*PerFertilized -0.603*PerUnconsolidated	0.085	0.610	4
9	0.490*Grasses -1.002*Shrubs -0.706*PerIntensiveUses - 0.848*Erosivity	0.084	0.609	4
10	0.568*Grasses -0.863*Shrubs -0.594*PerIntensiveUses + 0.223*PerMixIgSed + 0.199*PerCropping -0.876*Erosivity	0.062	0.699	6
	PP			
1	-0.344*Area + 1.149*MeanTP -0.363*PerUnconsolidated + 0.213*PerMixIgSed + 1.073*AnnTemp -1.550*ColdMonthTemp - 0.693*ColdQRain	0.065	0.794	7
2	1.26*MeanTP + 1.02*AnnTemp -2.37*ColdMonthTemp + 1.40*WarmQRain -1.08*ColdQRain	0.051	0.724	5
3	-0.409*Area + 0.977*MeanTP -0.416*PerUnconsolidated + 1.013*AnnTemp -1.562*ColdMonthTemp -0.654*ColdQRain	0.049	0.759	6
4	-0.445*Area + 1.253*MeanTP + 0.273*PerMixIgSed - 0.484*ColdMonthTemp + 0.820*HotMonthTemp - 0.675*ColdQRain	0.048	0.759	6
5	-0.443*Area + 0.861*MeanTP -0.361*PerUnconsolidated + 0.273*PerMixIgSed + 0.742*HotMonthTemp -0.932*AnnRain	0.048	0.759	6
6	1.166*MeanTP + 0.742*AnnTemp -2.201*ColdMonthTemp - 1.014*ColdQRain + 1.335*Erosivity	0.046	0.722	5
7	-1.063*Area + 1.050*MeanTP + 0.535*PerMixIgSed + 1.384*CatLength -0.916*MeanTN	0.044	0.721	5
8	1.098*MeanTP -0.336*PerUnconsolidated + 0.255*PerMixIgSed + 0.994*AnnTemp -1.307*ColdMonthTemp -0.518*ColdQRain	0.044	0.758	6
9	1.274*MeanTP + 0.287*PerMixIgSed + 0.820*AnnTemp - 1.182*ColdMonthTemp -0.543*ColdQRain	0.044	0.721	5
10	-0.761*Area + 0.973*MeanTP -0.348*PerUnconsolidated + 0.358*PerMixIgSed + 0.936*AnnTemp + 0.727*CatLength - 1.202*ColdMonthTemp -0.522*ColdQRain	0.042	0.816	8
11	-0.499*Area + 1.201*MeanTP + 0.284*PerMixIgSed - 0.461*AnnTemp + 1.232*HotMonthTemp -0.659*ColdQRain	0.040	0.756	6

12	-1.077*Area + 0.952*MeanTP -0.324*PerUnconsolidated + 0.485*PerMixIgSed + 1.294*CatLength -1.144*MeanTN	0.040	0.756	6
13	-1.012*Area + 0.735*MeanTP + 0.526*PerMixIgSed + 1.379*CatLength + 0.625*HotMonthTemp	0.039	0.719	5
14	1.088*MeanTP -0.314*PerUnconsolidated + 1.153*AnnTemp - 2.321*ColdMonthTemp + 1.202*WarmQRain -0.974*ColdQRain	0.037	0.755	6
15	-0.979*Area + 0.994*MeanTP + 0.530*PerMixIgSed + 1.171*CatLength + 0.658*HotMonthTemp -0.374*ColdQRain	0.037	0.755	6
16	-1.009*Area + 0.967*MeanTP -0.363*PerUnconsolidated + 0.469*PerMixIgSed + 1.102*CatLength + 0.484*HotMonthTemp - 0.822*MeanTN	0.037	0.787	7
17	-0.480*Area + 1.075*MeanTP -0.283*PerUnconsolidated + 0.242*PerMixIgSed -0.457*ColdMonthTemp + 0.923*HotMonthTemp -0.665*ColdQRain	0.036	0.787	7
18	1.017*MeanTP + 0.329*PerMixIgSed + 0.553*HotMonthTemp - 0.637*AnnRain	0.032	0.673	4
19	0.993*MeanTP + 0.338*PerMixIgSed + 0.666*HotMonthTemp + 0.530*pH	0.031	0.672	4
20	-0.314*Area + 1.334*MeanTP + 0.251*PerMixIgSed + 0.879*AnnTemp -1.395*ColdMonthTemp -0.704*ColdQRain	0.030	0.752	6
21	-0.901*Area + 0.909*MeanTP + 0.586*PerMixIgSed + 1.139*CatLength + 0.565*HotMonthTemp + 0.357*AnnRad	0.029	0.751	6
22	-0.369*Area + 1.094*MeanTP + 0.320*PerMixIgSed + 0.632*HotMonthTemp -0.920*AnnRain	0.028	0.714	5
23	-0.984*Area + 0.829*MeanTP -0.286*PerUnconsolidated + 0.485*PerMixIgSed + 1.104*CatLength + 0.772*HotMonthTemp - 0.382*ColdQRain	0.028	0.783	7
24	-0.538*Area + 1.059*MeanTP -0.330*PerUnconsolidated + 0.322*PerMixIgSed + 0.877*HotMonthTemp -0.668*WarmQRain - 0.427*ColdQRain	0.027	0.783	7
25	-0.476*Area + 1.034*MeanTP -0.356*PerUnconsolidated + 0.304*PerMixIgSed + 0.789*HotMonthTemp -0.313*ColdQRain - 0.772*AnnRain	0.025	0.782	7
26	0.777*MeanTP -0.520*PerUnconsolidated + 0.268*PerFertilized + 0.962*AnnTemp -1.331*ColdMonthTemp -0.543*ColdQRain	0.024	0.748	6
	EC			
1	-0.493*Mean_Elevation + 1.275*MeanCatSlope + 0.493*PerDrylandAgri + 0.364*PerCropping - 0.835*MeanCaExCap + 0.294*PerAcidS_B -0.417*MeanSoilEro - 2.413*AnnRain	0.182	0.837	8
2	-0.552*Mean_Elevation + 1.353*MeanCatSlope + 0.572*PerDrylandAgri + 0.354*PerCropping - 0.972*MeanCaExCap + 0.305*PerAcidS_B -0.486*MeanSoilEro - 3.023*AnnRain + 0.464*Mean_RR	0.137	0.856	9
3	-0.599*Mean_Elevation + 1.782*MeanCatSlope - 0.618*StreamDensity + 0.676*PerFertilized -1.018*MeanCaExCap -0.460*MeanSoilEro -2.733*AnnRain	0.106	0.806	7
4	-0.883*Mean_Elevation + 1.478*MeanCatSlope + 0.616*Forest + 0.756*PerFertilized -1.173*MeanCaExCap -0.639*MeanSoilEro - 3.747*AnnRain	0.095	0.805	7
5	-0.746*Mean_Elevation + 1.456*MeanCatSlope - 0.837*StreamDensity + 0.438*PerUrbanized -0.889*MeanCaExCap -0.357*MeanSoilEro -0.335*Bulk_density -2.449*AnnRain + 0.561*Mean_RR	0.092	0.852	9

6	-0.520*Mean_Elevation + 1.524*MeanCatSlope + 0.450*PerDrylandAgri + 0.490*PerCropping - 0.750*MeanCaExCap -0.442*MeanSoilEro -2.491*AnnRain	0.092	0.805	7
7	-0.426*Mean_Elevation + 1.507*MeanCatSlope -0.691*CatLength + 0.323*PerUrbanized -0.985*MeanCaExCap -0.387*Bulk_density -3.701*AnnRain -0.543*AnnRad	0.081	0.829	8
8	-0.672*Mean_Elevation + 1.394*MeanCatSlope - 0.733*StreamDensity + 0.345*PerUrbanized -0.893*MeanCaExCap + 0.223*PerAcidS_B -0.372*MeanSoilEro -0.369*Bulk_density - 2.559*AnnRain + 0.505*Mean_RR	0.074	0.870	10
9	-0.510*Mean_Elevation + 1.379*MeanCatSlope + 0.367*PerDrylandAgri + 0.311*PerCropping - 0.812*MeanCaExCap + 0.331*PerAcidS_B -0.414*MeanSoilEro - 0.167*Bulk_density -2.578*AnnRain	0.073	0.850	9
10	-0.728*Mean_Elevation + 1.634*MeanCatSlope - 0.880*StreamDensity + 0.403*PerUrbanized -0.255*Shrubs - 1.018*MeanCaExCap -0.364*MeanSoilEro -0.379*Bulk_density - 2.926*AnnRain + 0.611*Mean_RR	0.068	0.869	10

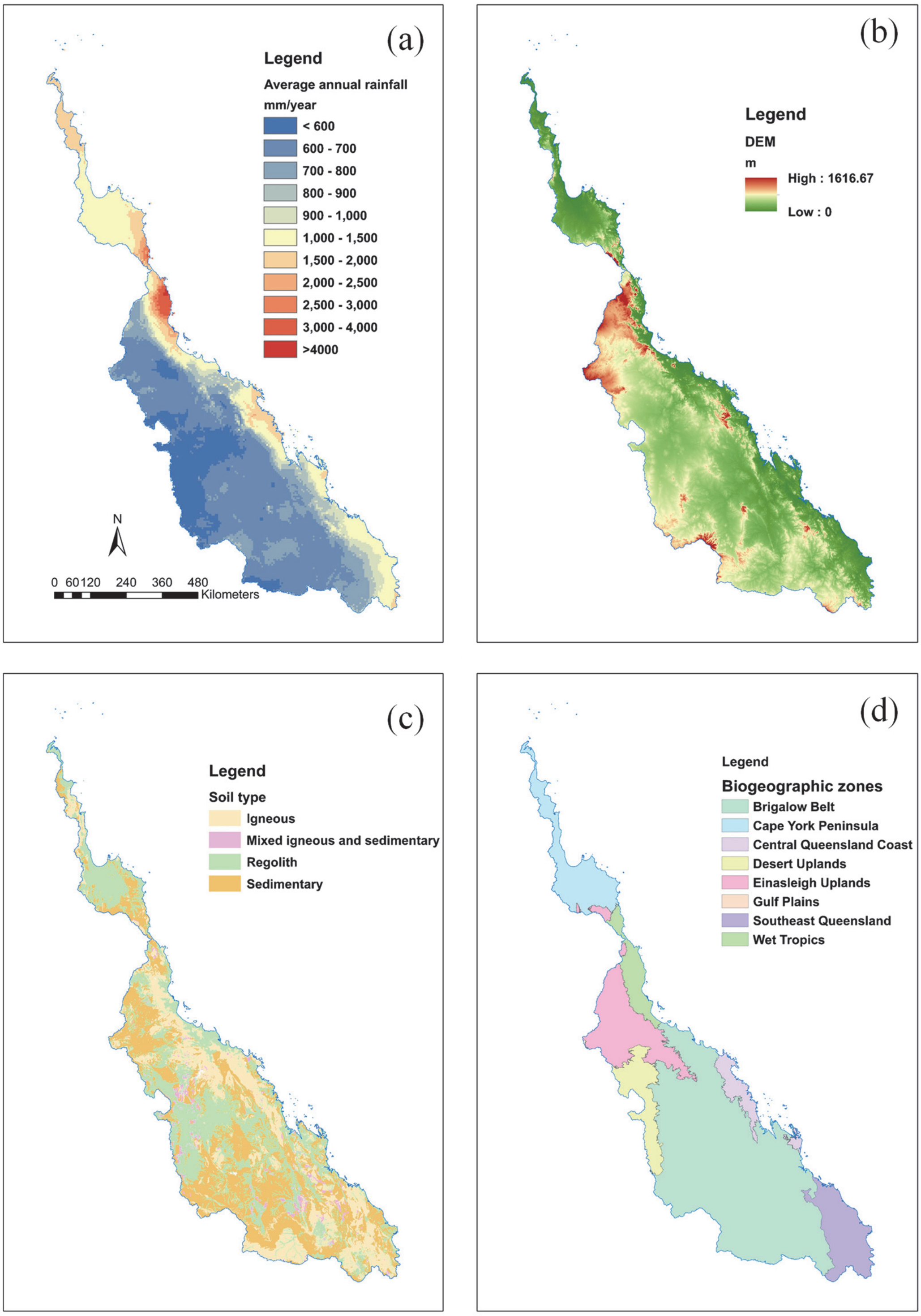

Figure S-7. Climatic, topographic, geological features of the GBR catchments: (a) average annual rainfall; (b) 250 m digital elevation model; (c) lithology type and (d) biogeographical bioregions. (Data sources - Australian Bureau of Meteorology (2016); Geoscience Australia (2008); Australian Soil Resource Information System (2011); Department of Environment and Science-Queensland Government (2010)).

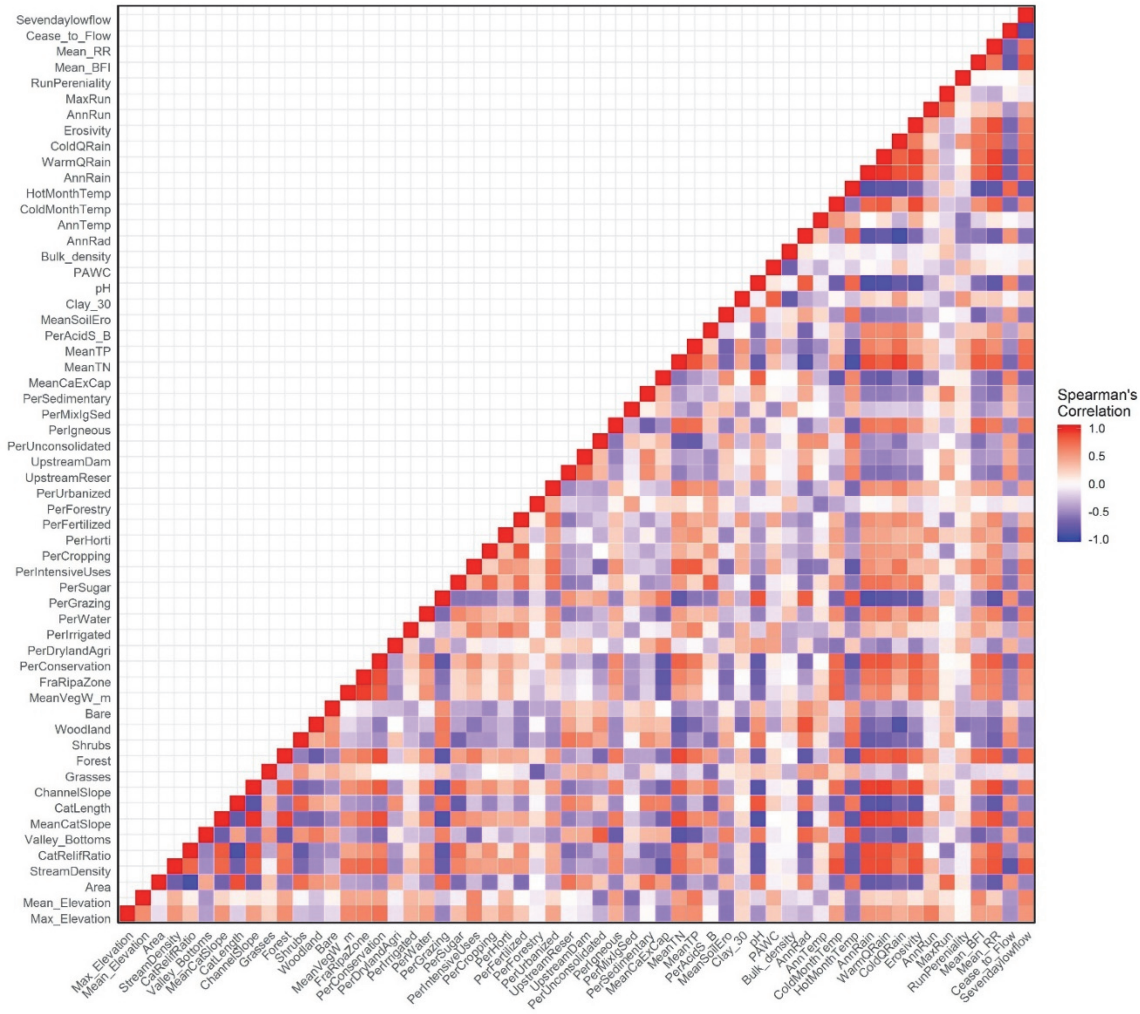

Figure S-8. Cross-correlation heatmap of all 58 catchment characteristics. See Table S-13 for more details of these catchment characteristics.

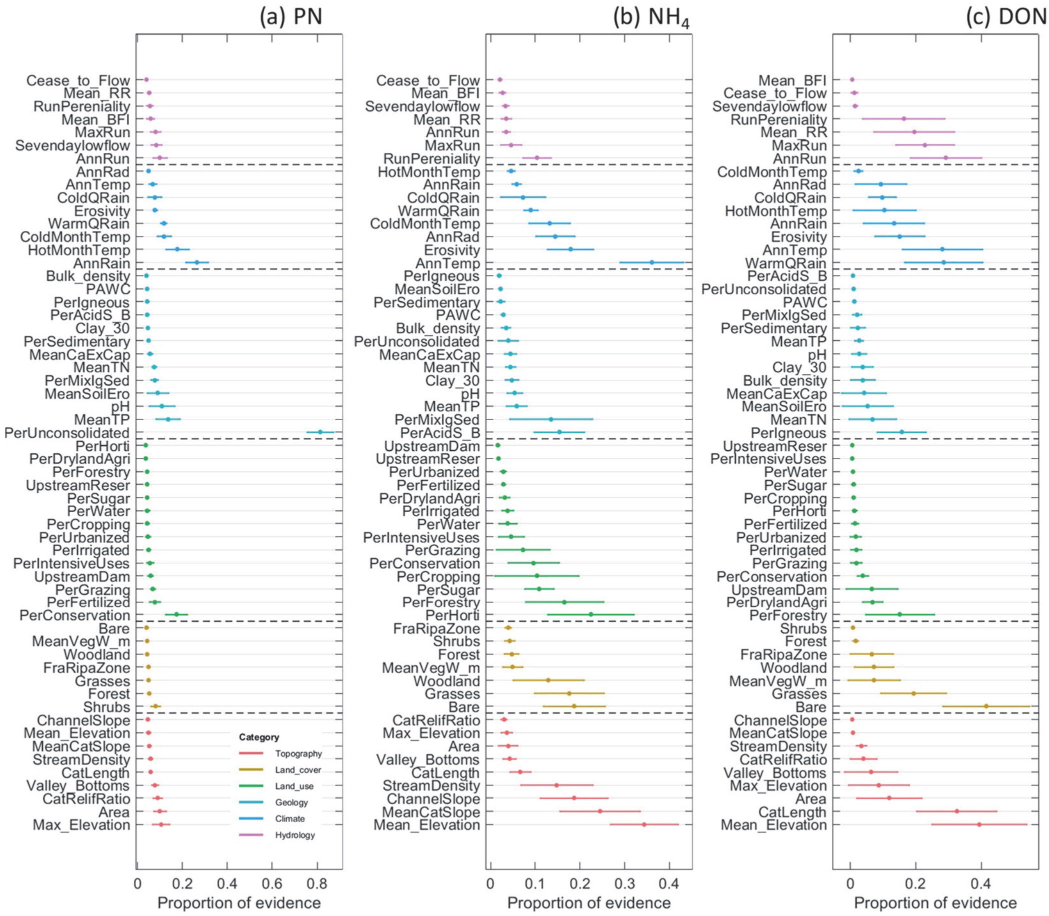

Figure S-9. Proportion of Evidence (PoE) of each catchment characteristics for: (a) PN; (b) NH_4 and (c) DON. Dot represents the average of PoE from 20 subsampling tests, with horizontal bar indicates the ± one standard deviation. Catchment characteristics within each category (represented by six different colours, see legend in panel a) were plotted in a descending order of the corresponding average PoE. The definition of abbreviation of each catchment characteristic can be found in Table S-13.

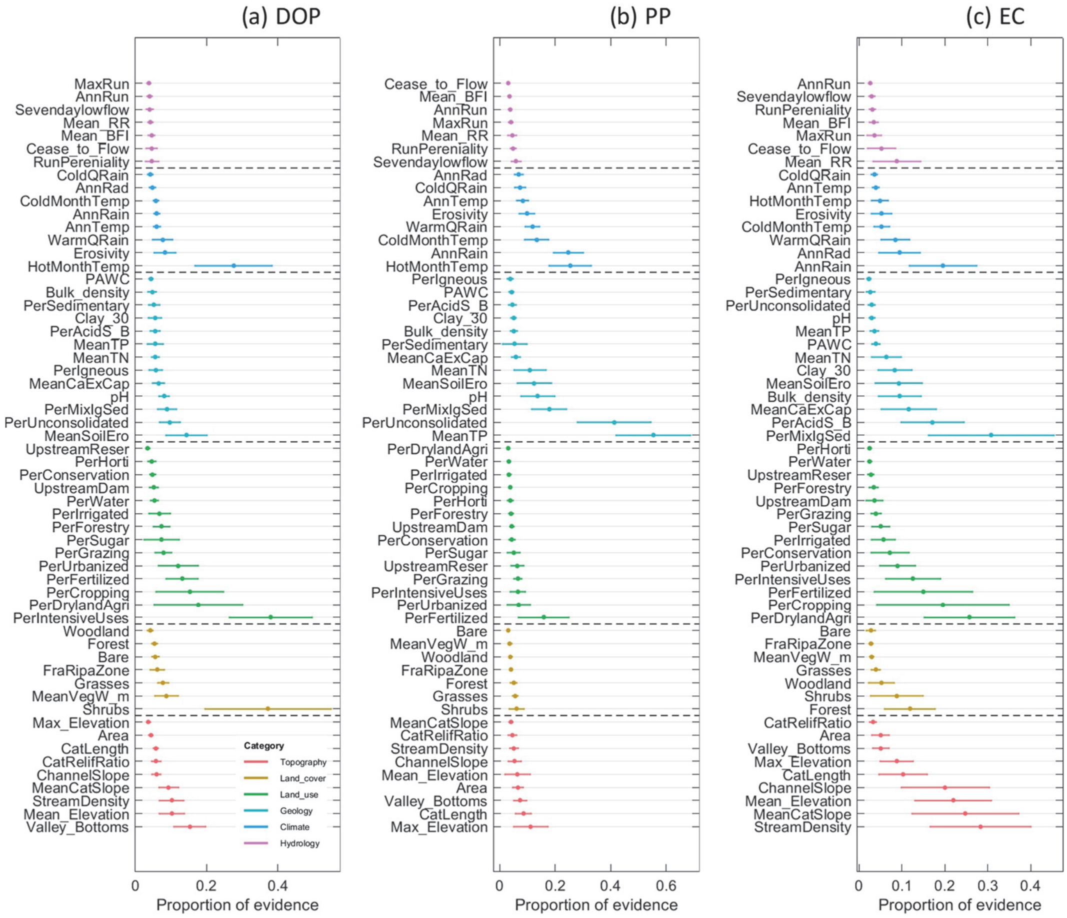

Figure S-10. Proportion of Evidence (PoE) of each catchment characteristics for: (a) DOP; (b) PP and (c) EC. Dot represents the average of PoE from 20 subsampling tests, with horizontal bar indicates the ± one standard deviation. Catchment characteristics within each category (represented by six different colours, see legend in panel a) were plotted in a descending order of the corresponding average PoE. The definition of abbreviation of each catchment characteristic can be found in Table S-13.

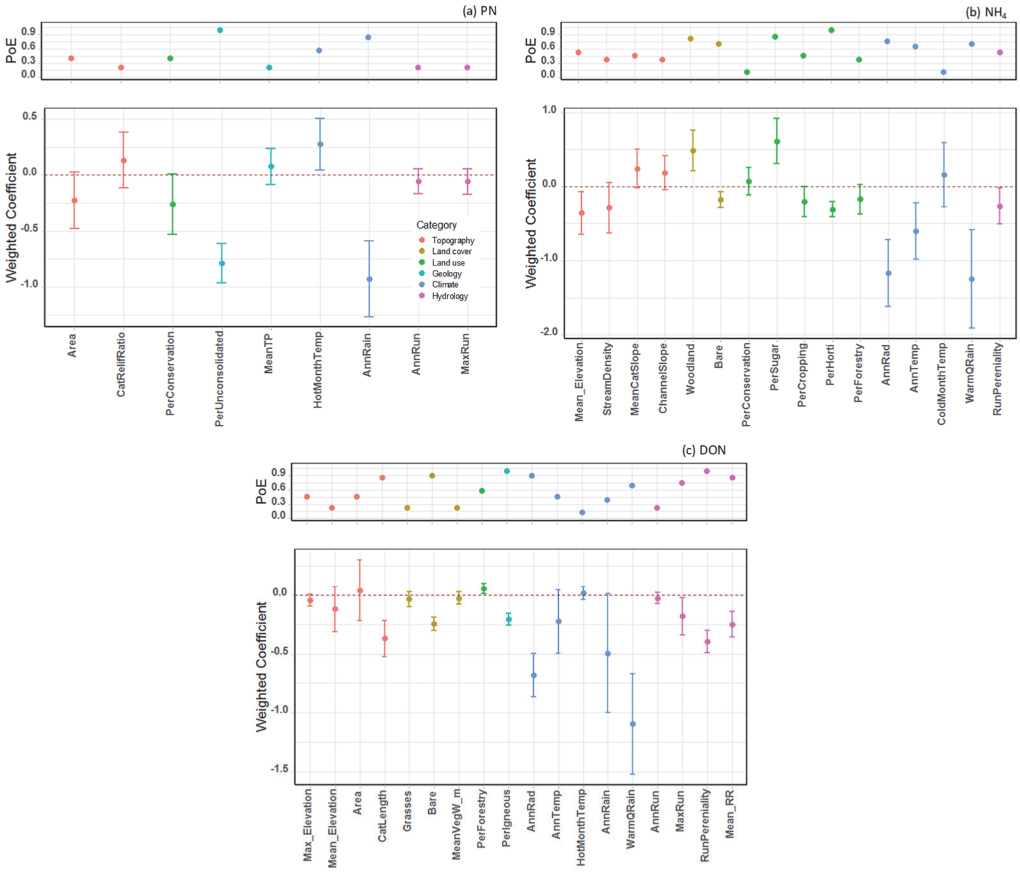

Figure S-11. Weighted coefficients and Proportion of Evidence (PoE) of catchment characteristics selected in the final plausible models for: (a) PN; (b) NH_4 and (c) DON. Bottom panel indicated the mean (dot, $\overline{\beta}_j$, Equation 5-4) and standard deviation (error bar, $var(\overline{\beta}_j)$, Equation 5-5) of each selected catchment characteristics, and different colour represents each category (see legend in panel a). The PoE was calculated based on model Akaike weights across all final plausible models.

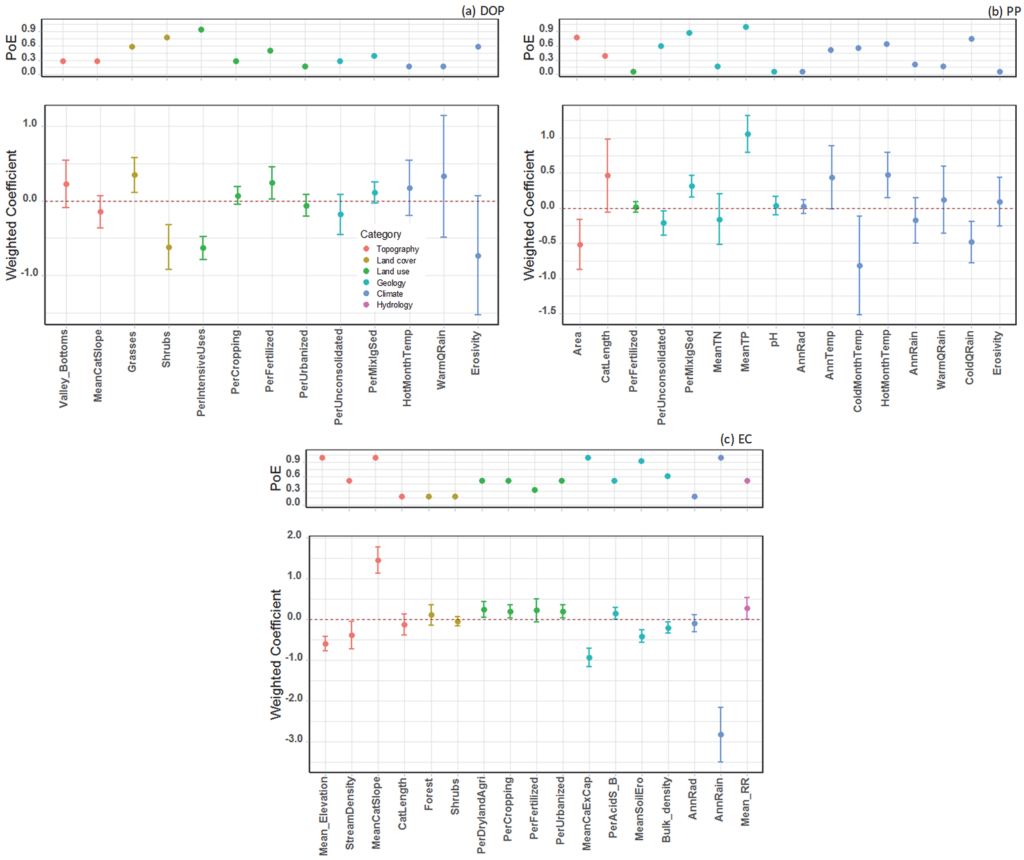

Figure S-12. Weighted coefficients and Proportion of Evidence (PoE) of catchment characteristics selected in the final plausible models for: (a) DOP; (b) PP and (c) EC. Bottom panel indicated the mean (dot, $\overline{\beta}_j$, Equation 5-4) and standard deviation (error bar, $var(\overline{\beta}_j)$, Equation 5-5) of each selected catchment characteristics, and different colour represents each category (see legend in panel a). The PoE was calculated based on model Akaike weights across all final plausible models.

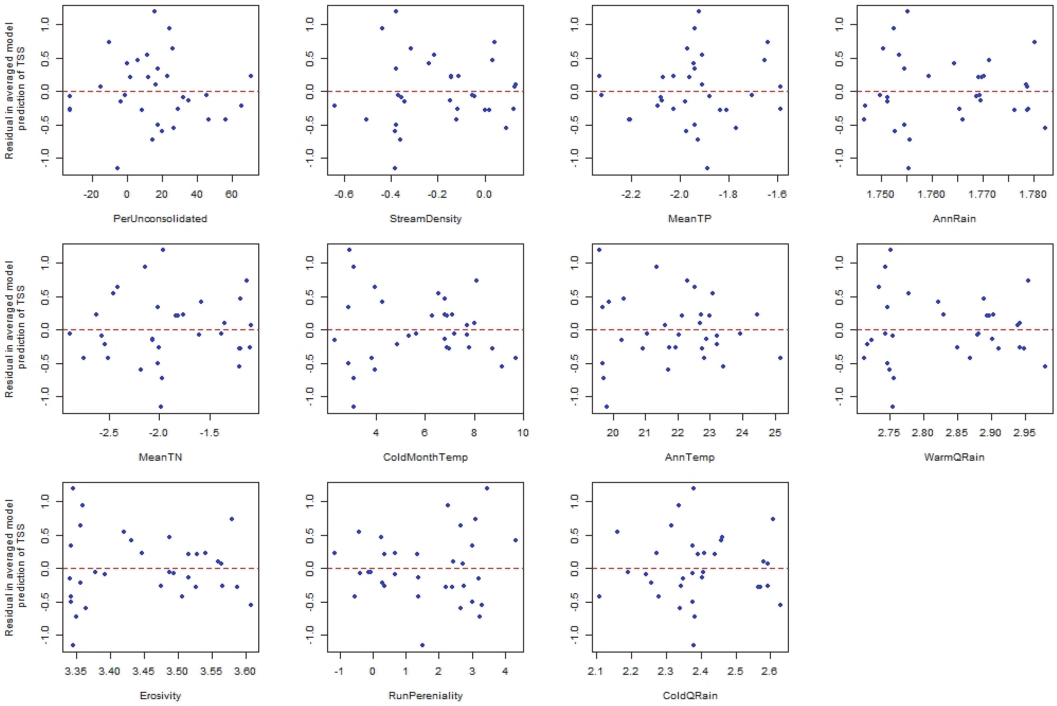

Figure S-13. Relationship between residual in averaged prediction of TSS and catchment characteristics included in the final plausible models.

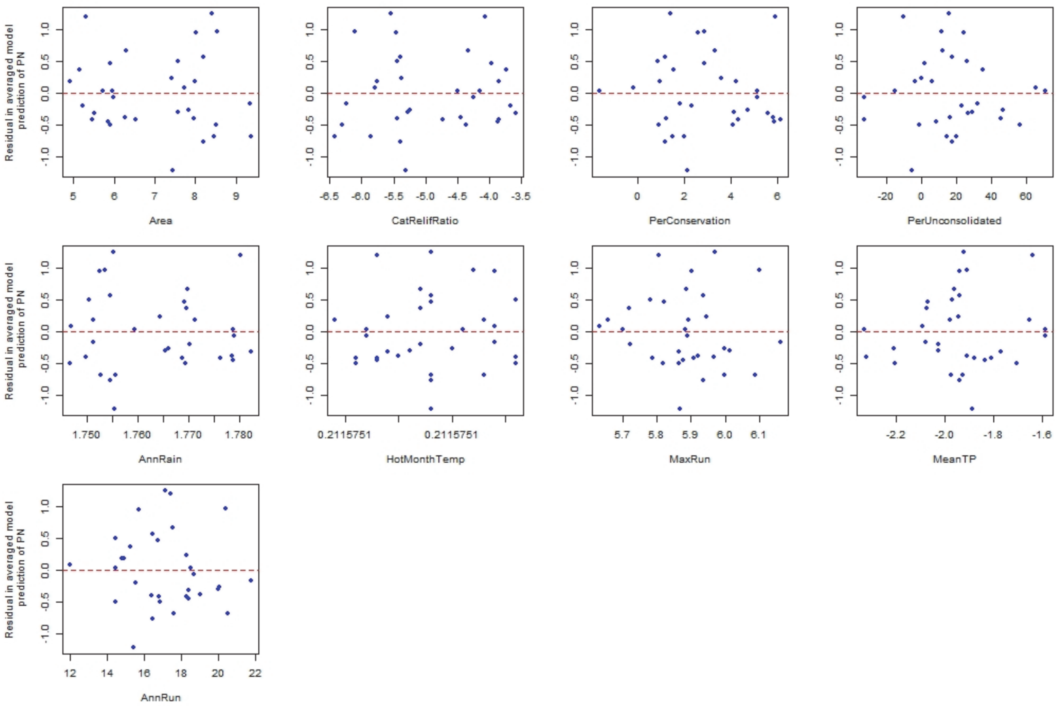

Figure S-14. Relationship between residual in averaged prediction of NO_X and catchment characteristics included in the final plausible models

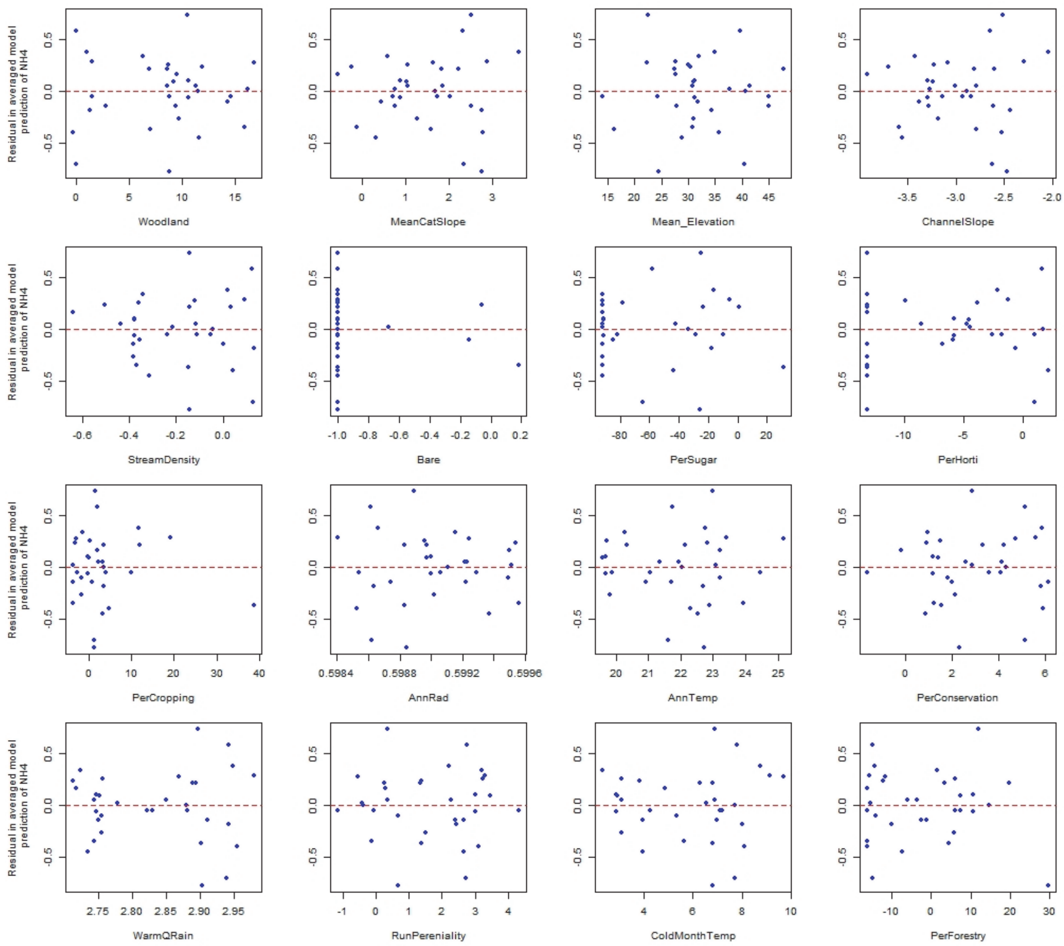

Figure S-15. Relationship between residual in averaged prediction of NH_4 and catchment characteristics included in the final plausible models.

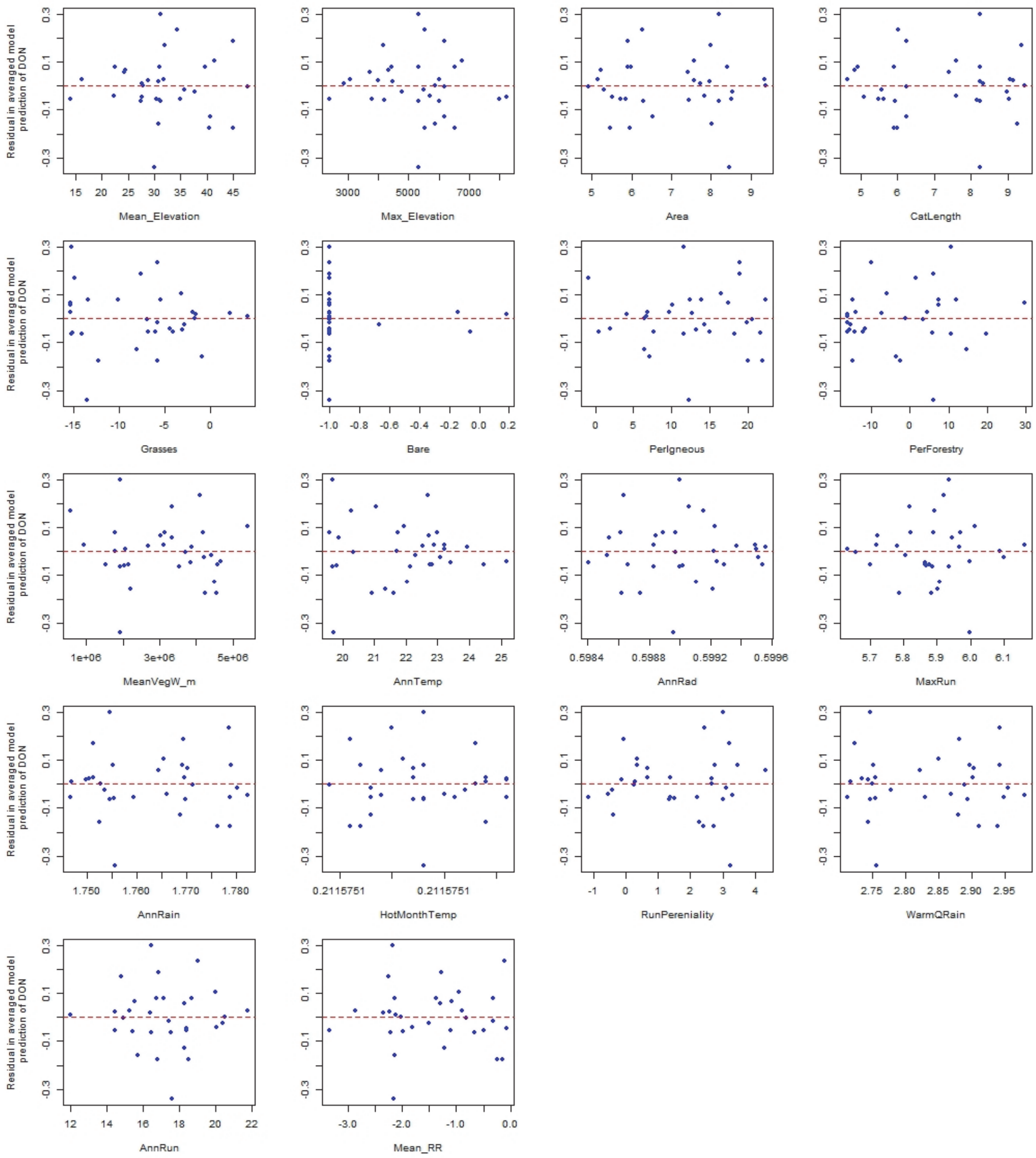

Figure S-16. Relationship between residual in averaged prediction of DON and catchment characteristics included in the final plausible models.

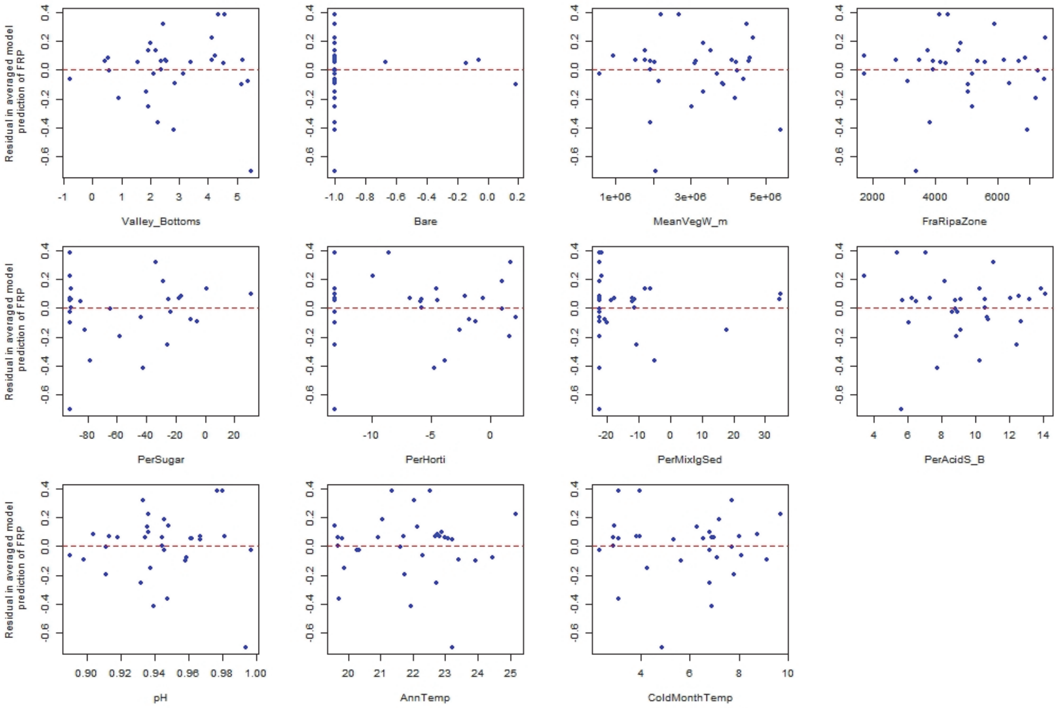

Figure S-17. Relationship between residual in averaged prediction of FRP and catchment characteristics included in the final plausible models.

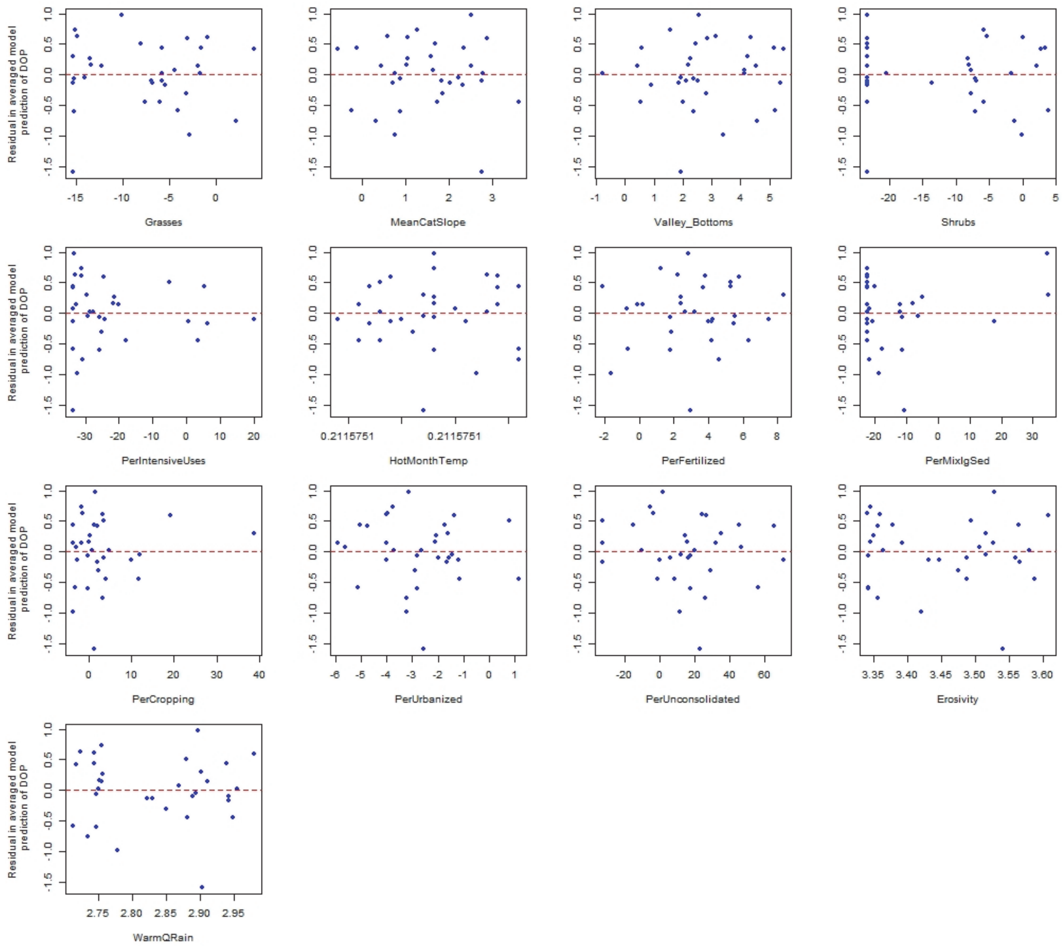

Figure S-18. Relationship between residual in averaged prediction of DOP and catchment characteristics included in the final plausible models.

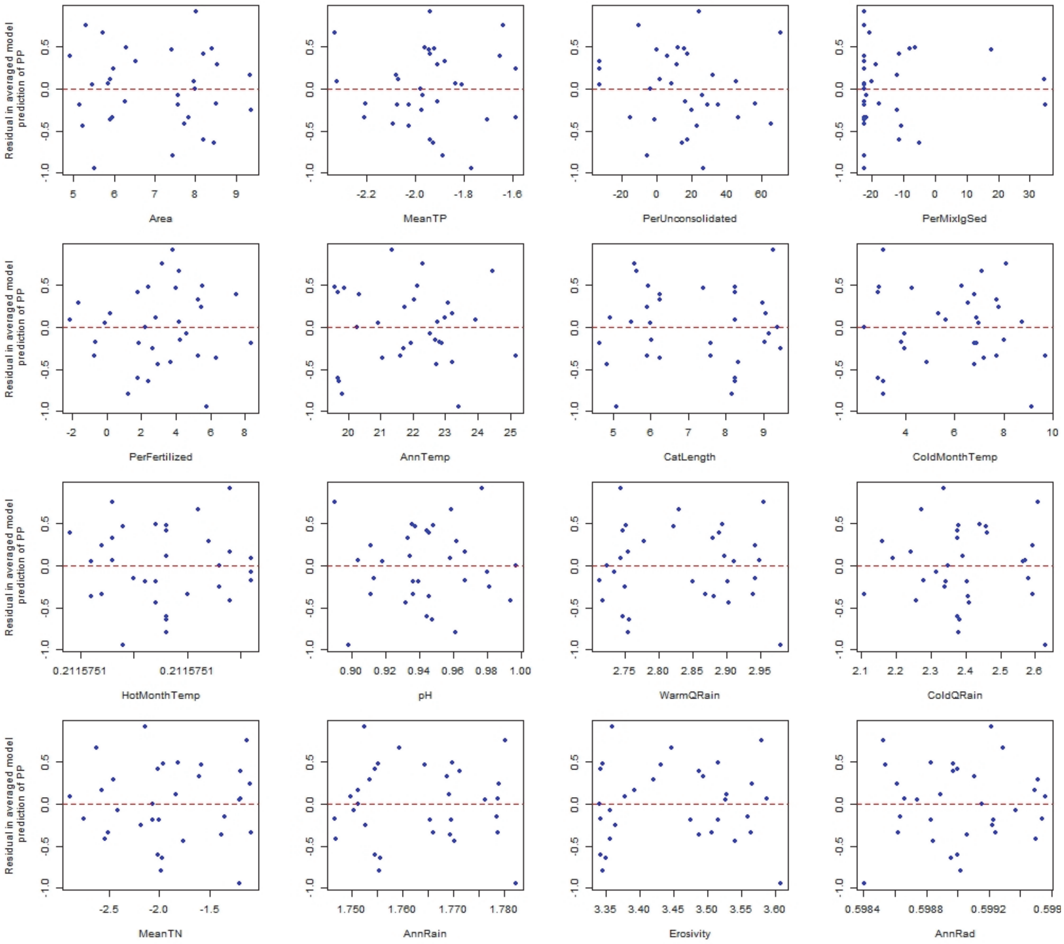

Figure S-19. Relationship between residual in averaged prediction of PP and catchment characteristics included in the final plausible models.

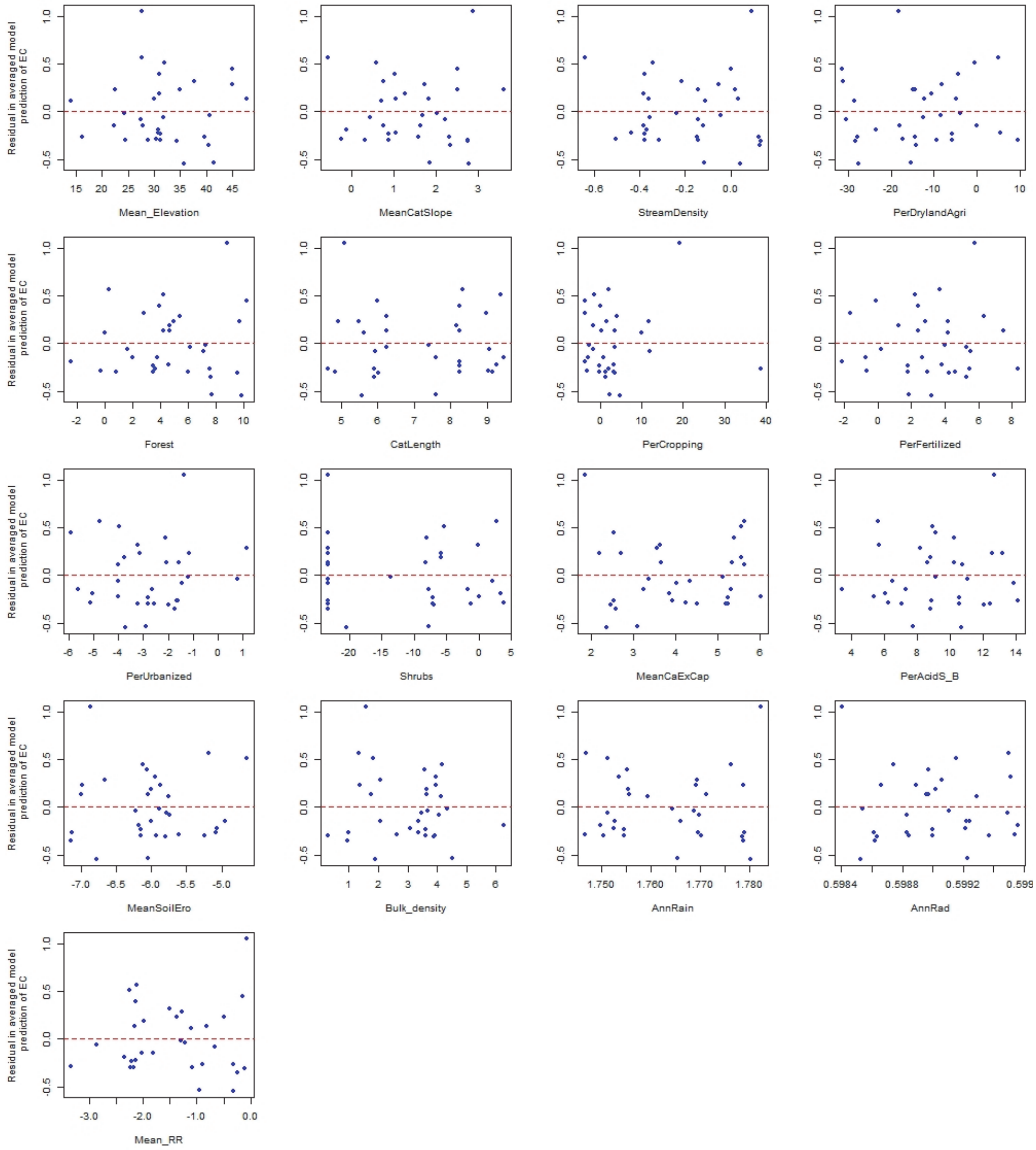

Figure S-20. Relationship between residual in averaged prediction of EC and catchment characteristics included in the final plausible models.

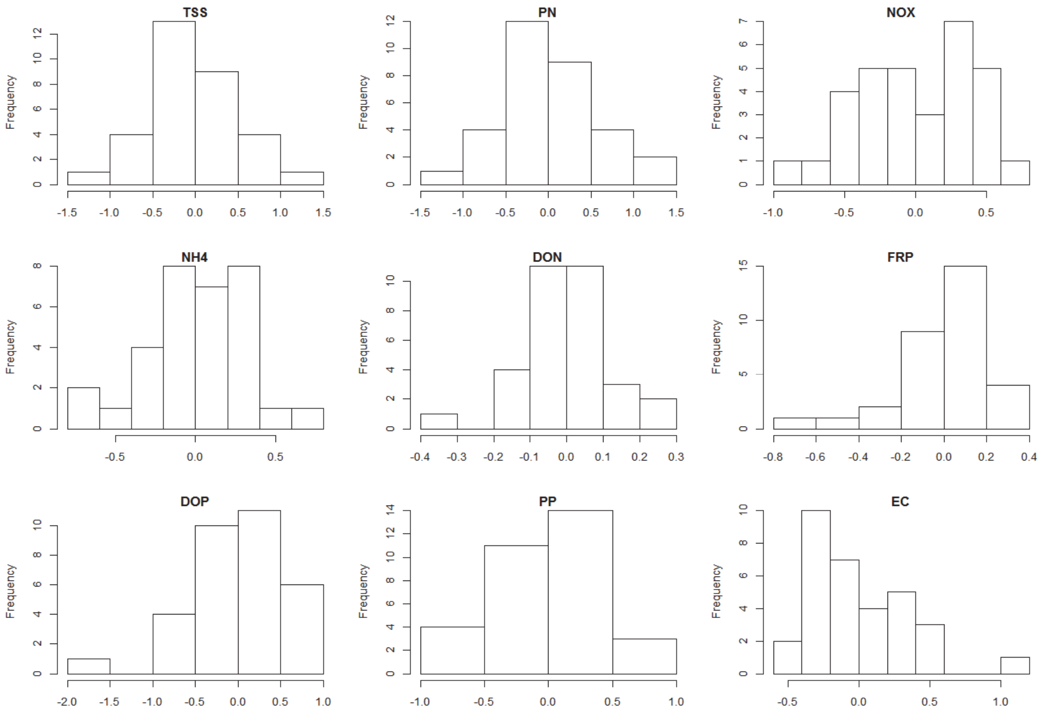

Figure S-21. Histograms showing distribution of residuals of nine constituents from averaged model predictions.

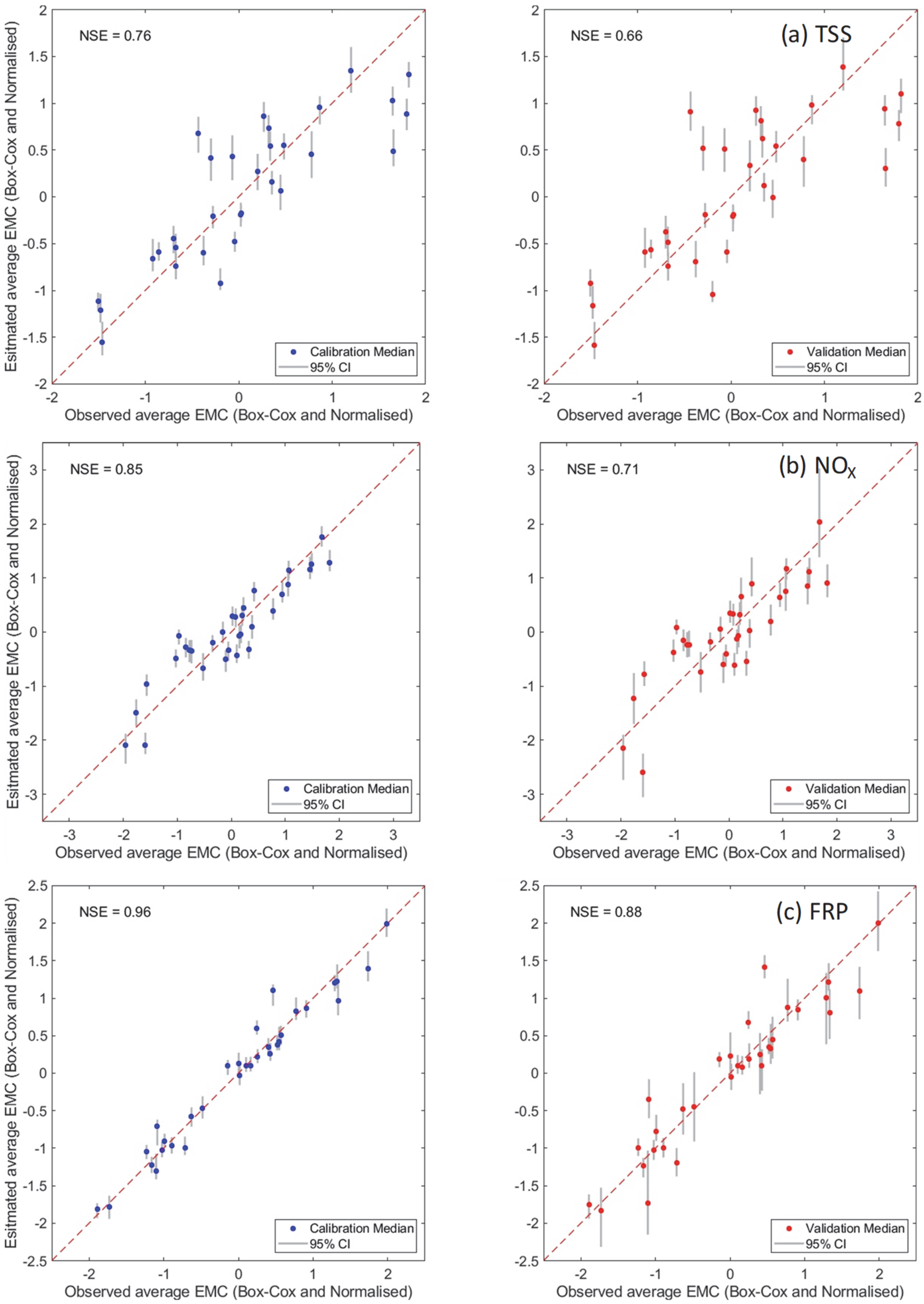

Figure S-22. Observed and estimated average EMC for: (a) TSS; (b) NO_X and (c) FRP. Results derived from 5,000 time subsampling five-fold cross-validation: plots with blue dots and red dots represent calibration and validation results, respectively. The grey bar represents the 95% confident interval. NSE was calculated based on median value of predictions of each site.

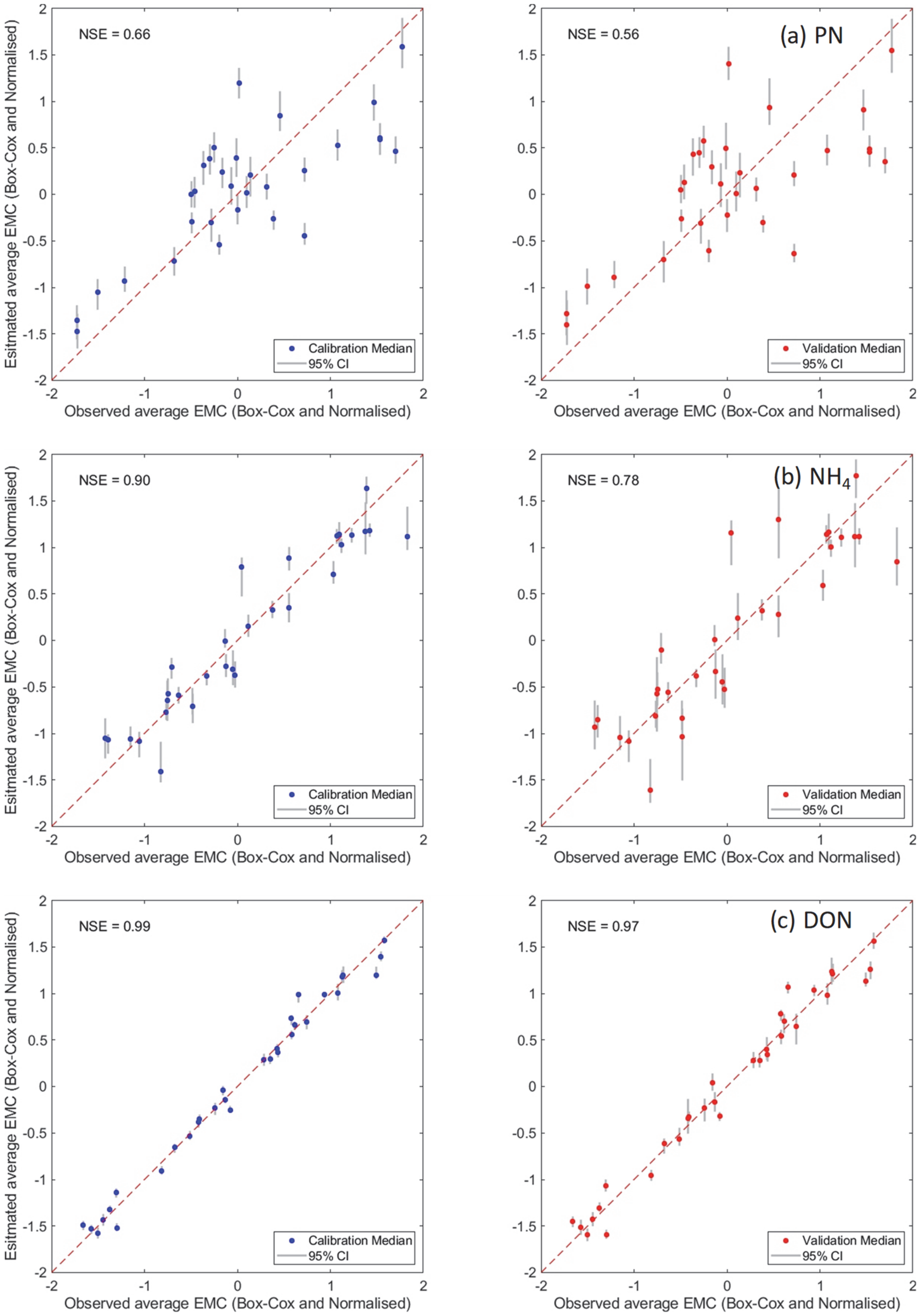

Figure S-23. Observed and estimated average EMC for: (a) PN; (b) NH_4 and (c) DON. Results derived from 5,000 time subsampling five-fold cross-validation: plots with blue dots and red dots represent calibration and validation results, respectively. The grey bar represents the 95% confident interval. NSE was calculated based on median value of predictions of each site.

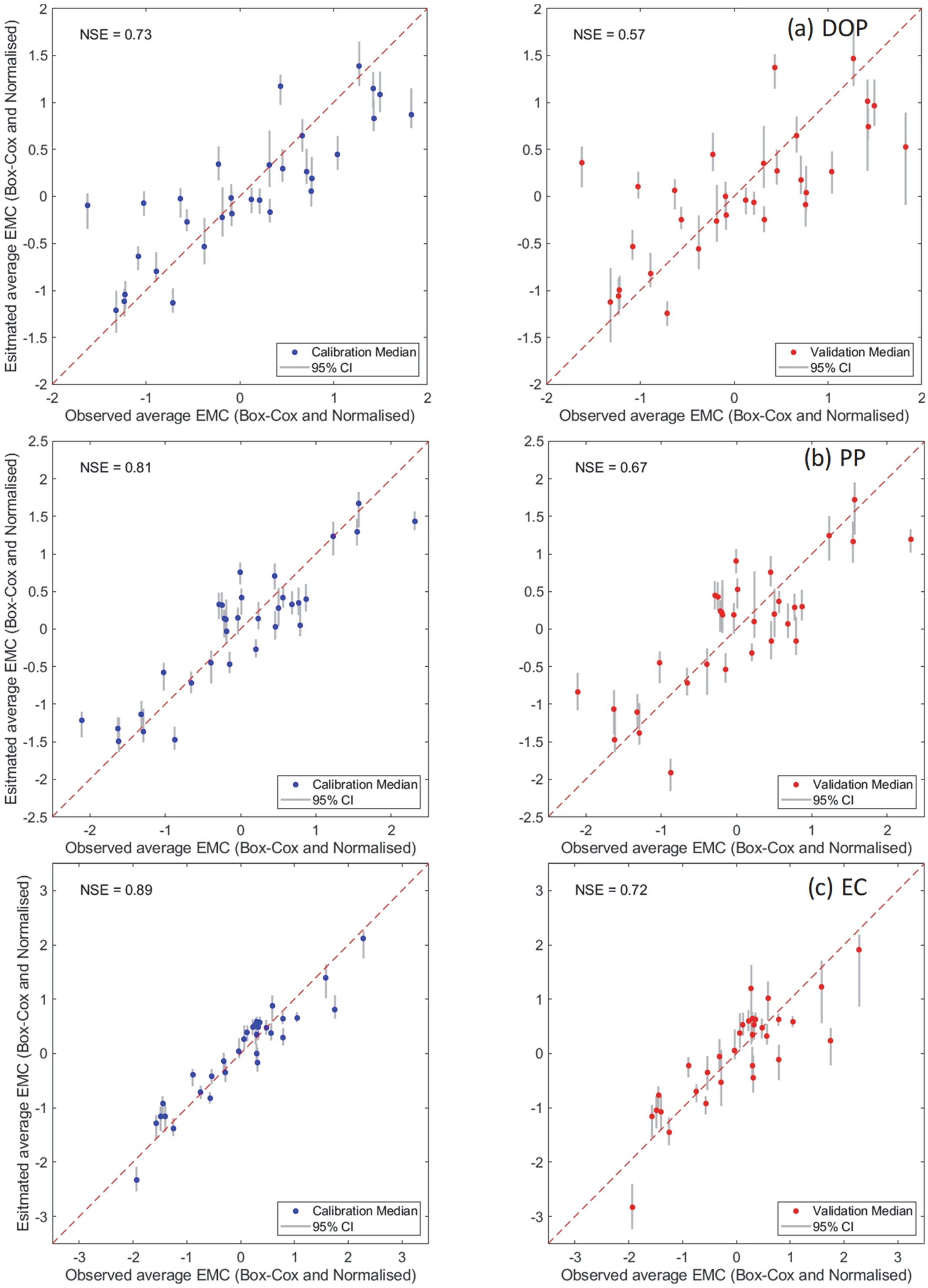

Figure S-24. Observed and estimated average EMC for: (a) DOP; (b) PP and (c) EC. Results derived from 5,000 time subsampling five-fold cross-validation: plots with blue dots and red dots represent calibration and validation results, respectively. The grey bar represents the 95% confident interval. NSE was calculated based on median value of predictions of each site.

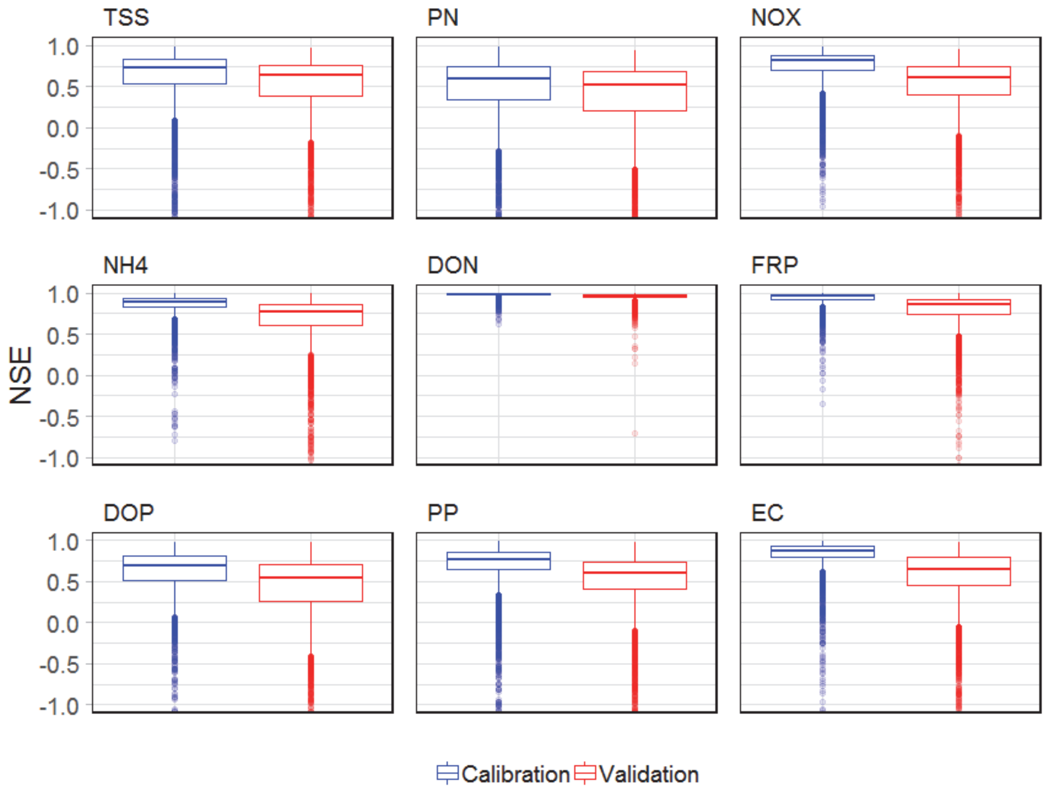

Figure S-25. Comparison distribution of NSEs between calibration and validation results based on 5,000 times subsampling cross-validation.

A3. Supplementary Materials for Chapter 6

Table S-17. Number of EMCs for each constituent

Cluster	TSS	PN	NO_X	NH_4	DON	FRP	DOP	PP	EC
One	225	207	218	217	215	210	66	186	174
Two	381	370	372	370	373	372	231	366	354
% of event monitored	43	41	42	42	42	41	21	39	37

Table S-18. Posterior inclusion probability of individual predictor derived from BMA on two clusters of sites.

Predictor	TSS		PN		NO_X		NH_4		DON		FRP		DOP		PP		EC	
	Cluster one	Cluster two	Cluster one	Cluster two	Cluster one	Cluster two	Cluster one	Cluster two	Cluster one	Cluster two	Cluster one	Cluster two	Cluster one	Cluster two	Cluster one	Cluster two	Cluster one	Cluster two
Event_ave_Q	**0.87**	0.52	**0.86**	0.40	**0.96**	0.44	0.26	0.68	0.50	0.44	0.35	0.42	0.46	0.60	**0.87**	**0.86**	**1.00**	0.57
Event_max_Q	**0.84**	**1.00**	0.76	**1.00**	0.33	0.72	0.17	**0.81**	0.79	0.63	**0.95**	0.57	0.46	**0.83**	0.75	**1.00**	**1.00**	0.55
Event_ave_P	**0.87**	**0.92**	**0.94**	**0.83**	0.37	0.09	0.34	0.59	0.55	0.18	**0.81**	**0.87**	0.48	0.20	**0.83**	**0.80**	0.67	0.43
Event_max_P	0.32	0.55	0.33	0.23	0.64	0.01	0.14	0.16	0.35	0.17	0.73	0.51	0.43	0.30	0.77	0.15	0.45	0.67
Event_T	0.10	0.37	0.34	0.16	0.21	**0.97**	0.20	0.63	**0.82**	0.25	0.78	**0.80**	0.48	0.79	0.40	0.61	0.61	**0.81**
Event_NDVI	0.05	0.33	0.14	0.77	**0.83**	0.24	0.71	0.64	0.41	0.34	0.38	0.55	0.50	**0.96**	0.44	0.50	**1.00**	**1.00**
Event_SM	0.40	0.21	0.73	0.54	0.78	0.28	**0.91**	0.24	0.62	0.19	0.63	0.38	0.43	0.72	0.34	0.40	0.45	**0.83**
Event_AET	0.21	0.09	0.20	0.93	0.51	**1.00**	0.63	0.55	0.41	**0.84**	0.51	0.25	0.51	**0.83**	0.20	**0.81**	0.67	0.35
Ante_Q	0.18	0.20	0.75	**0.86**	0.16	**1.00**	0.33	0.36	0.58	0.27	0.36	**0.89**	0.48	0.18	0.31	0.12	**1.00**	**1.00**
Ante_P	0.12	0.08	0.17	0.05	0.20	0.04	0.28	0.72	0.25	0.77	0.25	**0.86**	0.49	**0.96**	0.16	0.07	**0.85**	0.19
Ante_NDVI	0.34	**1.00**	0.58	**1.00**	**0.92**	**1.00**	**0.99**	**0.89**	0.54	**1.00**	**0.97**	**0.88**	0.66	**1.00**	0.56	**1.00**	0.67	0.58
Ante_SM	0.19	0.76	0.47	**0.94**	0.75	**1.00**	0.70	**0.96**	**0.85**	**0.99**	**0.90**	**0.96**	0.46	**0.85**	0.21	0.59	0.67	0.42
Ante_AET	0.14	0.69	0.36	0.28	0.32	**0.95**	0.28	0.71	0.41	0.09	0.38	0.53	0.41	0.32	0.18	0.63	0.49	**1.00**
Post_Q	**0.88**	0.13	0.68	0.31	0.19	**1.00**	0.21	0.76	0.58	**0.84**	0.18	0.75	0.42	0.17	0.29	0.36	**1.00**	**1.00**
Post_P	**0.92**	0.01	0.79	0.06	0.17	**0.91**	0.19	0.22	0.42	0.07	0.25	0.37	0.42	0.10	0.75	0.02	0.67	**1.00**
Post_SM	0.23	0.04	0.24	0.40	**0.95**	0.65	0.45	0.27	0.39	0.13	0.43	0.28	0.47	0.22	0.23	0.11	0.33	**1.00**
Post_AET	0.26	0.13	0.26	0.03	0.27	0.77	0.34	0.37	0.54	0.25	0.36	**0.97**	0.42	0.54	0.27	0.22	0.67	0.04

Note: Posterior inclusion probability >= 0.8 in bold and red

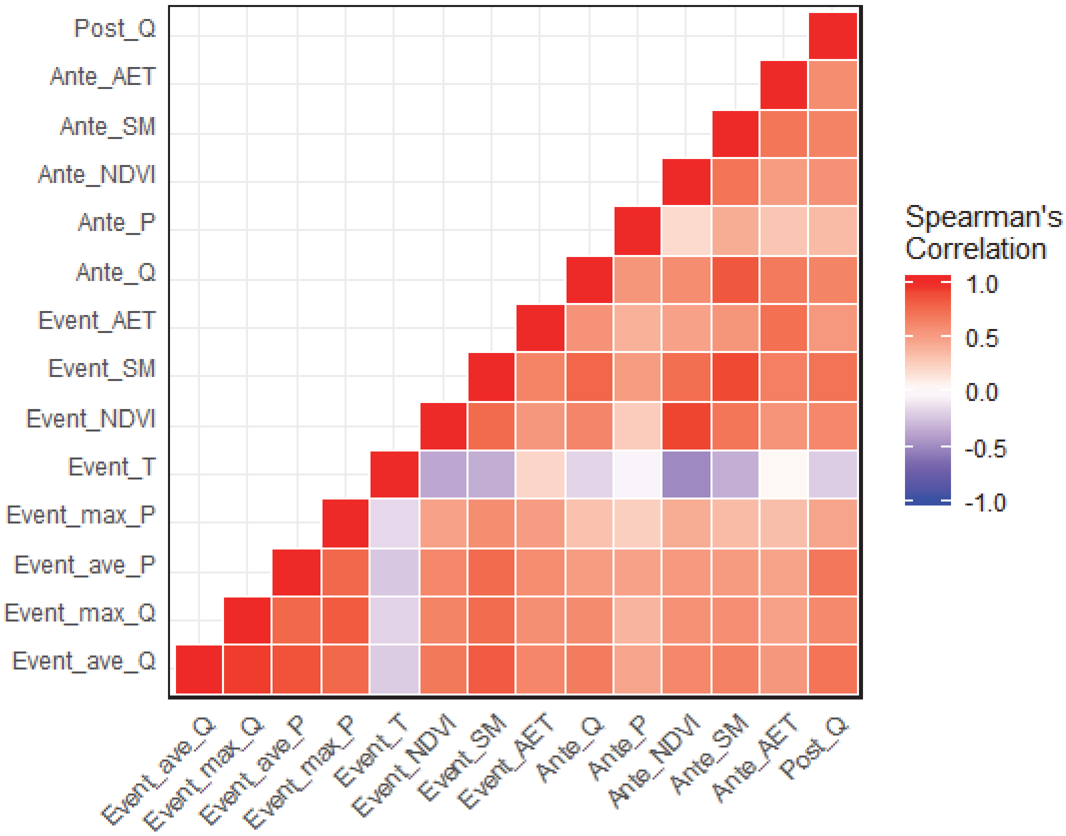

Figure S-26. Spearman's Rank correlation between 14 candidate predictors.

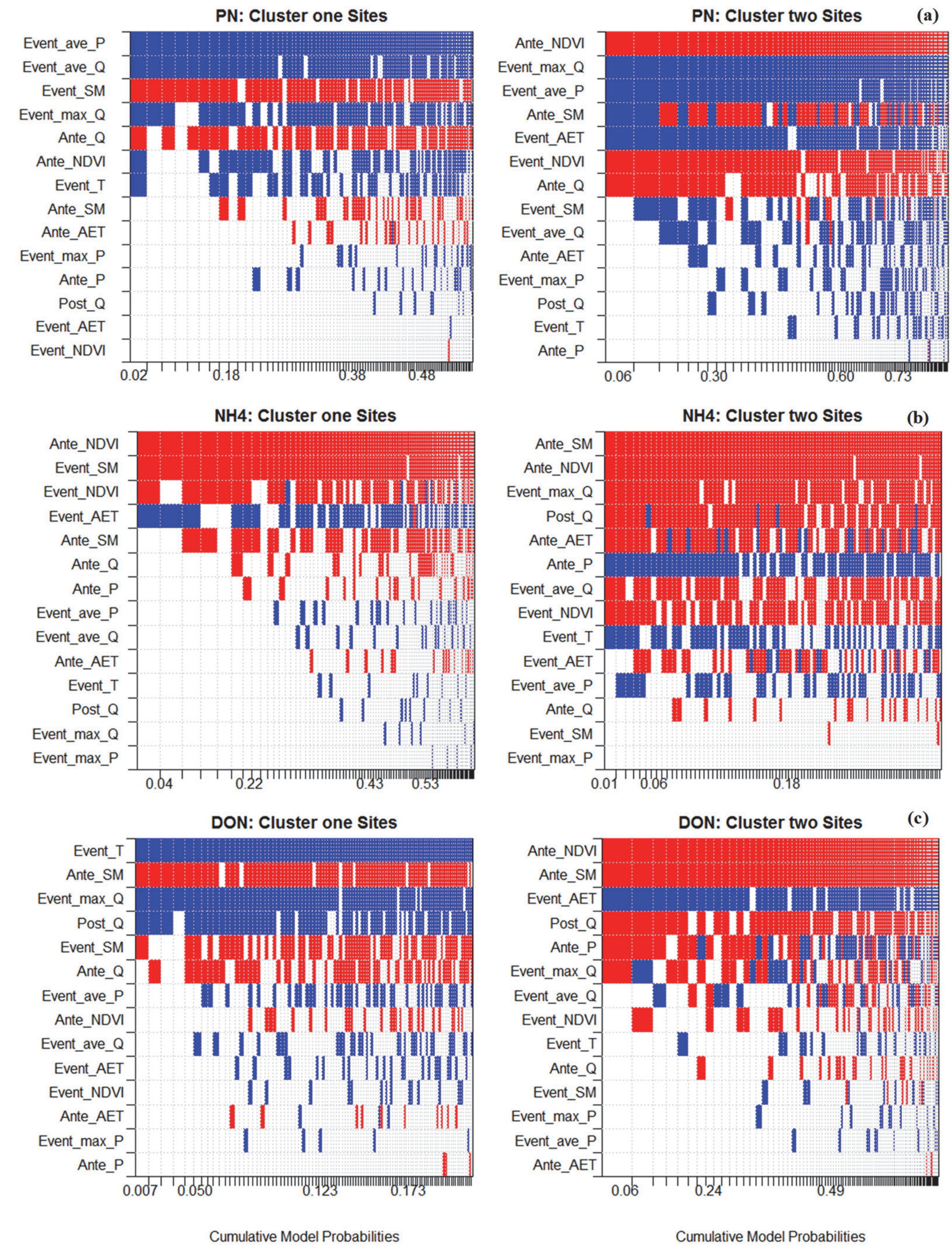

Figure S-27. Comparison of BMA model coefficient and cumulative model probability (only the top 100 models are shown) between two clusters for: (a) PN, (b) NH_4 and (c) DON. Left - cluster one sites and Right – cluster two sites. The order of predictors on the y-axis was ranked based on the posterior inclusion probability. Each column in the heatmap represents the one specific model (ranked from highest model probability) and the width of the column is normalised by the posterior model probability. The colour indicates the direction of the coefficients, red – negative and blue – positive. Note: the coefficient value was averaged across the posterior median value of site-specific coefficient within each cluster (effect size, $\theta_{n,j}$, in Equation 6-5).

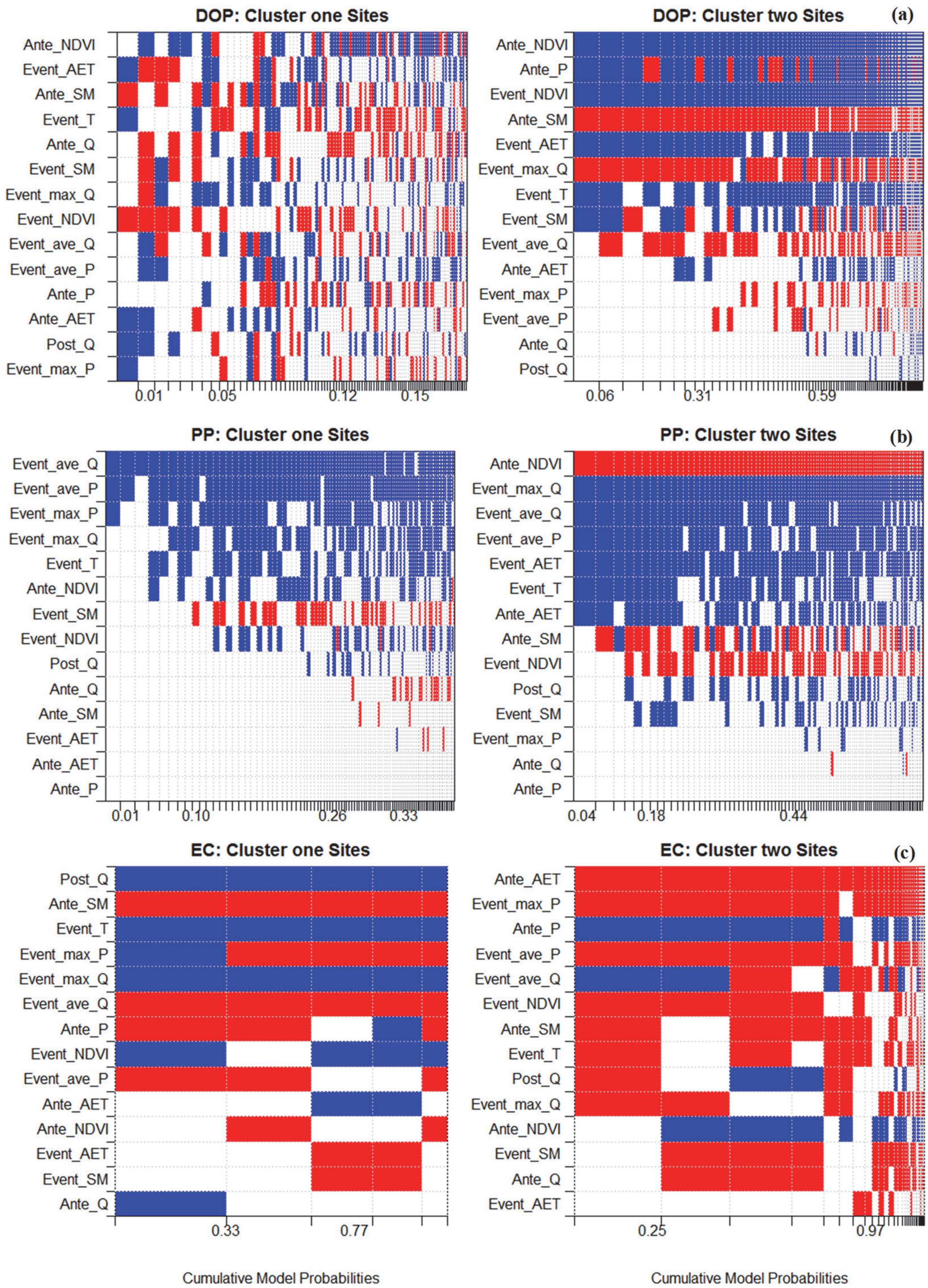

Figure S-28. Comparison of BMA model coefficient and cumulative model probability (only the top 100 models are shown) between two clusters for: (a) DOP, (b) PP and (c) EC. Left - cluster one sites and Right – cluster two sites. The order of predictors on the y-axis was ranked based on the posterior inclusion probability. Each column in the heatmap represents the one specific model (ranked from highest model probability) and the width of the column is normalised by the posterior model probability. The colour indicates the direction of the coefficients, red – negative and blue – positive. Note: the coefficient value was averaged across the posterior median value of site-specific coefficient within each cluster (effect size, $\theta_{n,j}$, in Equation 6-5).

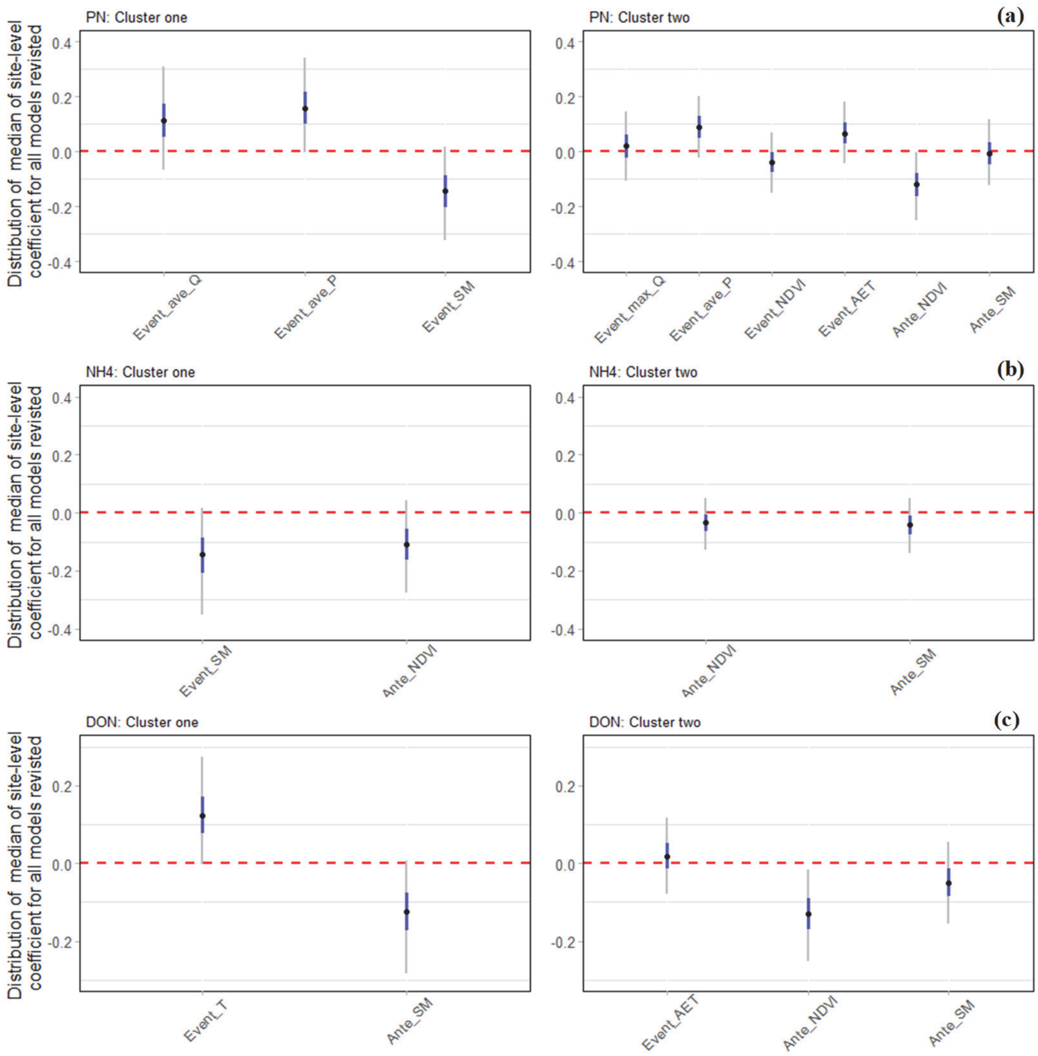

Figure S-29. Distribution of median of site-level coefficients for all plausible models in BMA. (a) PN, (b) NH_4 and (c) DON. Only predictors with PIP > 0.8 are included. For each specific model structure, the coefficient value of a predictor was the median of site-specific coefficient across all sites (effect size, $\theta_{n,j,}$ in Equation 6-5). The distribution of this value thus represents the probability of the model (PMP), as well as variability in the same predictor across different sites. Note: black dots indicate the median; grey vertical lines indicate 95% CI and blue coloured vertical lines indicates 50% CI. The definition of abbreviation of each predictor can be found in Table 6-3.

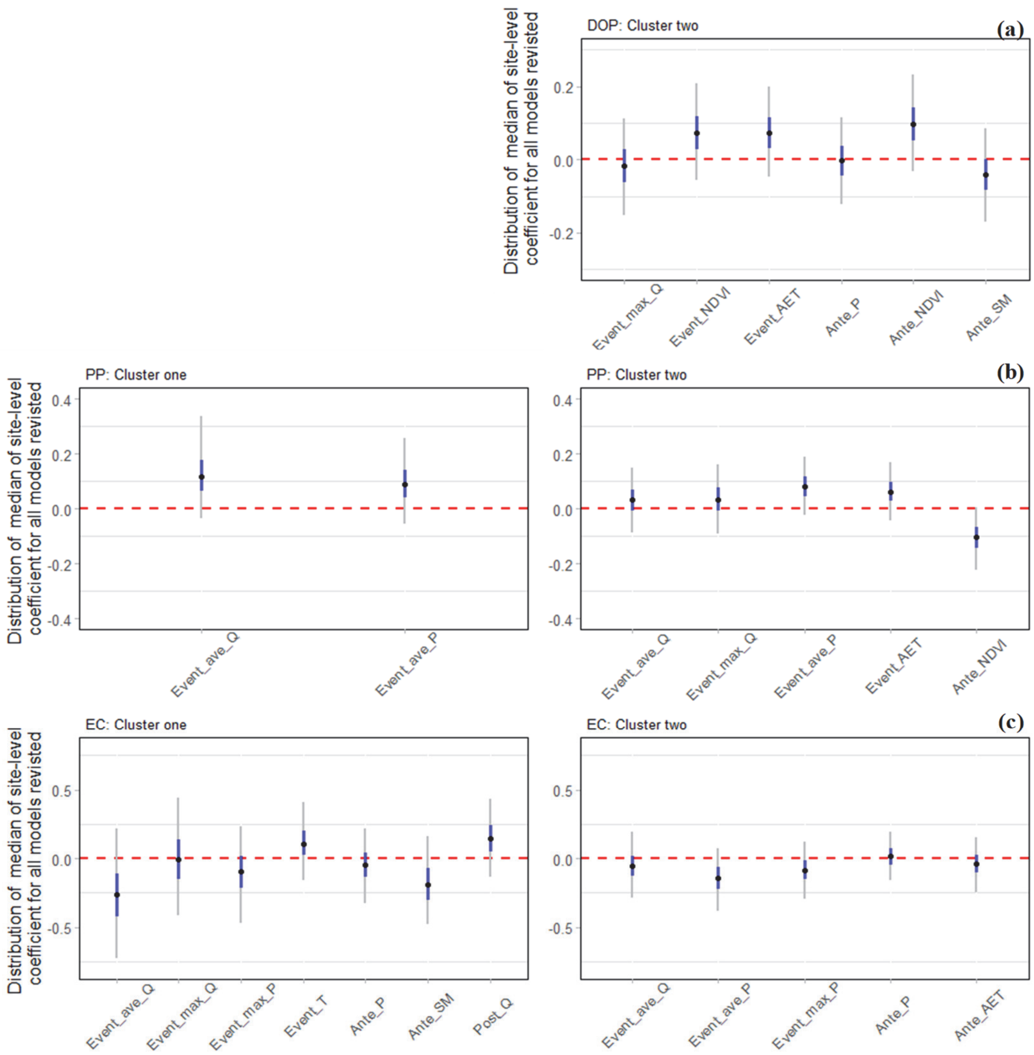

Figure S-30. Distribution of median of site-level coefficients for all plausible models in BMA. (a) DOP, (b) PP and (c) EC. Only predictors with PIP > 0.8 are included. For each specific model structure, the coefficient value of a predictor was the median of site-specific coefficient across all sites (effect size, $\theta_{n,j,}$ in Equation 6-5). The distribution of this value thus represents the probability of the model (PMP), as well as variability in the same predictor across different sites. Note: black dots indicate the median; grey vertical lines indicate 95% CI and blue coloured vertical lines indicates 50% CI. The definition of abbreviation of each predictor can be found in Table 6-3.

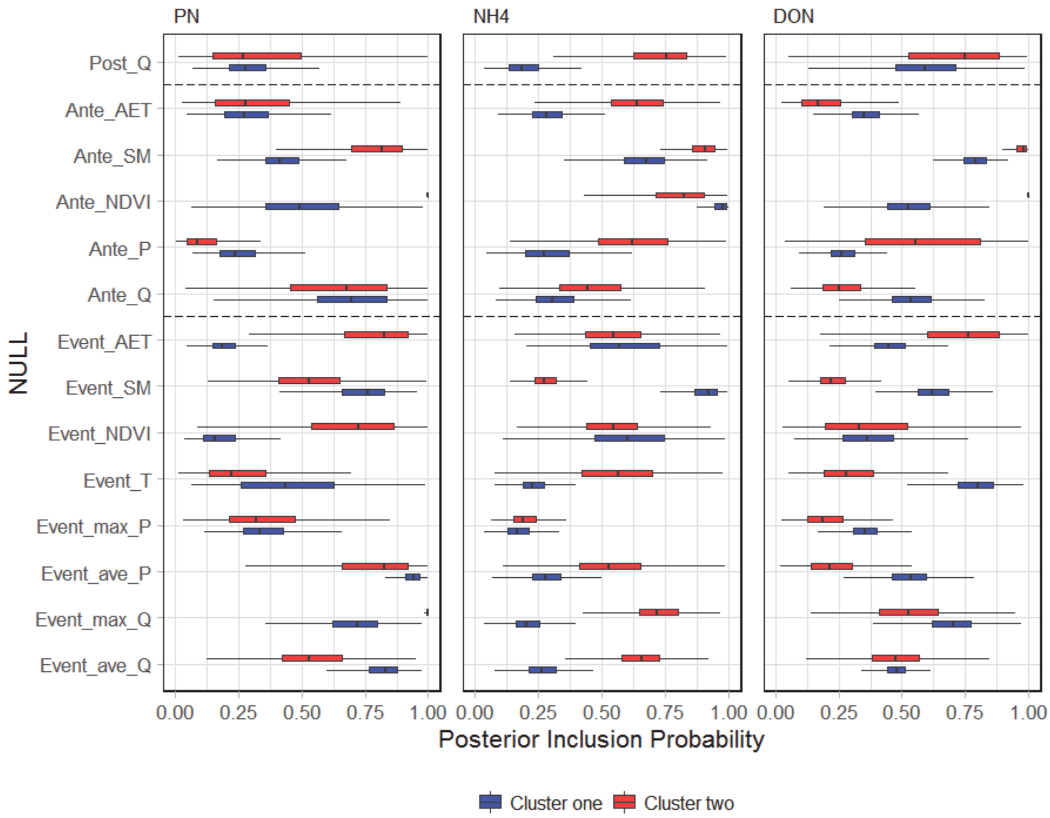

Figure S-31. The comparisons of distribution of posterior inclusion probability of individual predictors derived from 1,000 subsampled BMA runs. Note: colour represents different clusters: blue - Cluster and red - Cluster two. The definition of abbreviation of each predictor can be found in Table 6-3.

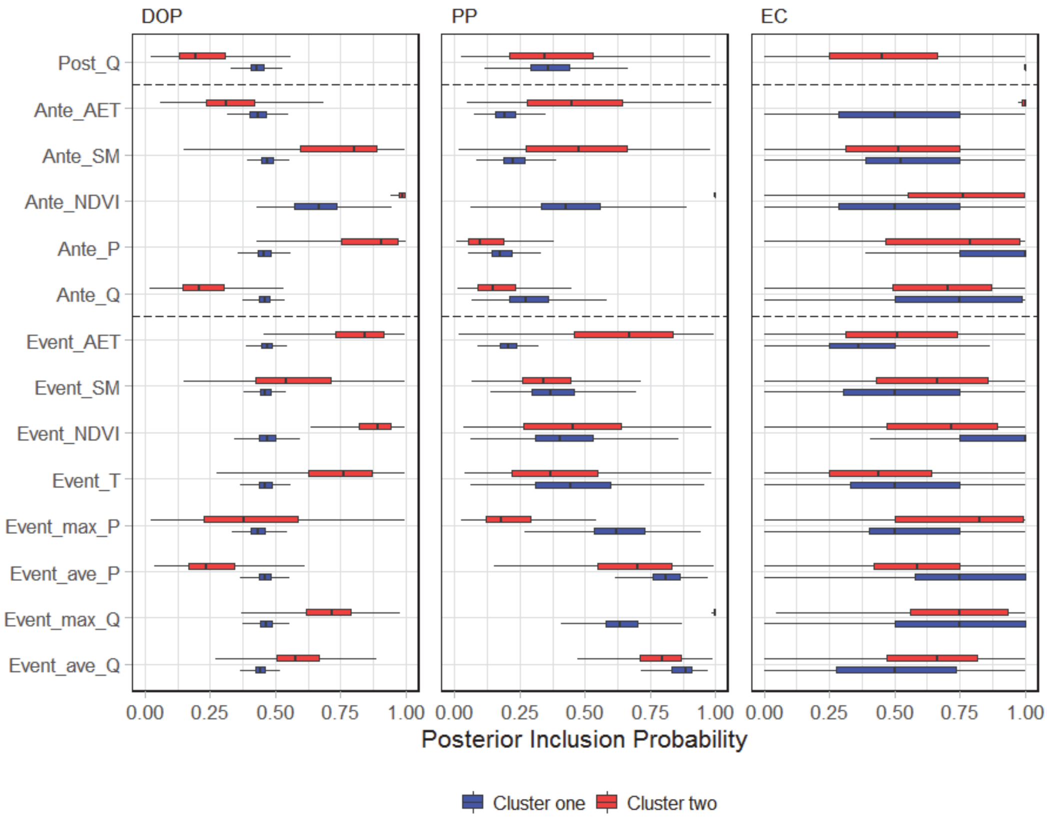

Figure S-32. The comparisons of distribution of posterior inclusion probability of individual predictors derived from 1,000 subsampled BMA runs. Note: colour represents different clusters: blue - Cluster and red - Cluster two. The definition of abbreviation of each predictor can be found in Table 6-3.

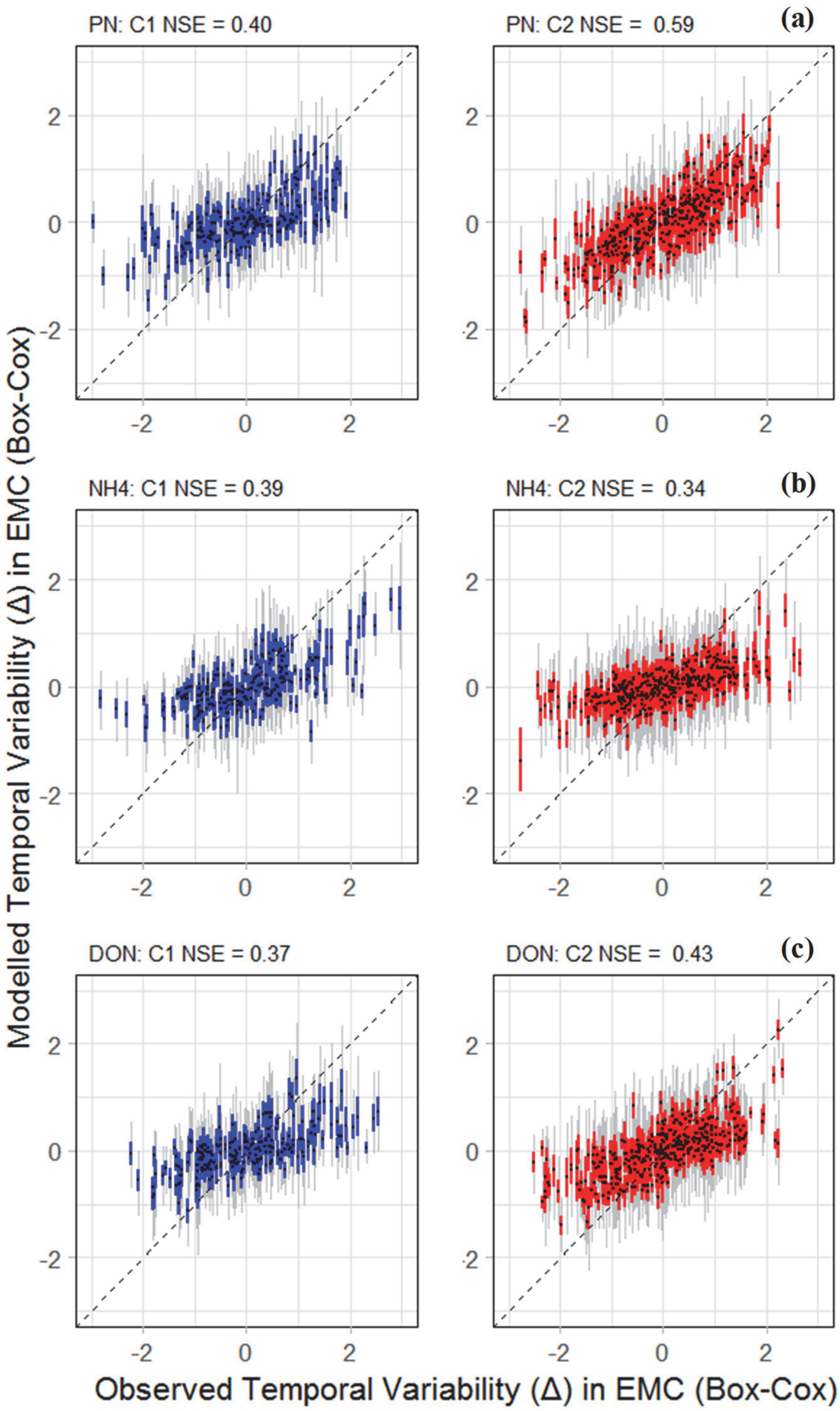

Figure S-33. Performance of the BMA models of the temporal variability of nine constituents across 32 sites, represented by prediction intervals from BMA and observed Box-Cox EMC across two clusters of sites for: (a) PN; (b) NH_4 and (c) DON. The NSE values are calculated based on predictions within group- (cluster) level. Note: black dots are the prediction median; grey vertical lines are the 95% CI and coloured vertical lines indicates 50% CI: blue - Cluster and red - Cluster two. The dashed black lines is the 1:1 relationship.

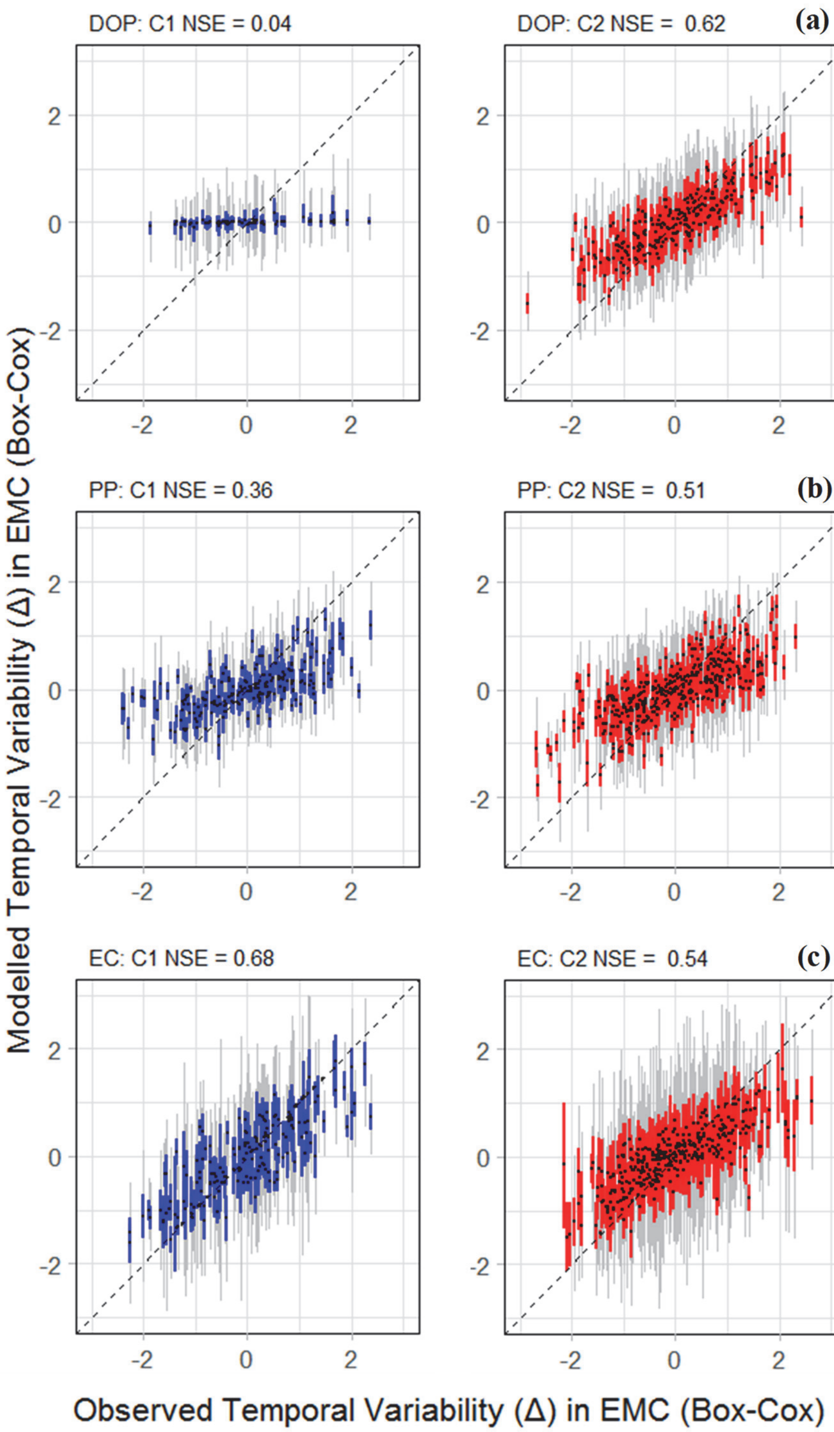

Figure S-34. Performance of the BMA models of the temporal variability of nine constituents across 32 sites, represented by prediction intervals from BMA and observed Box-Cox EMC across two clusters of sites for: (a) DOP; (b) PP and (c) EC. The NSE values are calculated based on predictions within group- (cluster) level. Note: black dots are the prediction median; grey vertical lines are the 95% CI and coloured vertical lines indicates 50% CI: blue - Cluster and red - Cluster two. The dashed black lines is the 1:1 relationship.

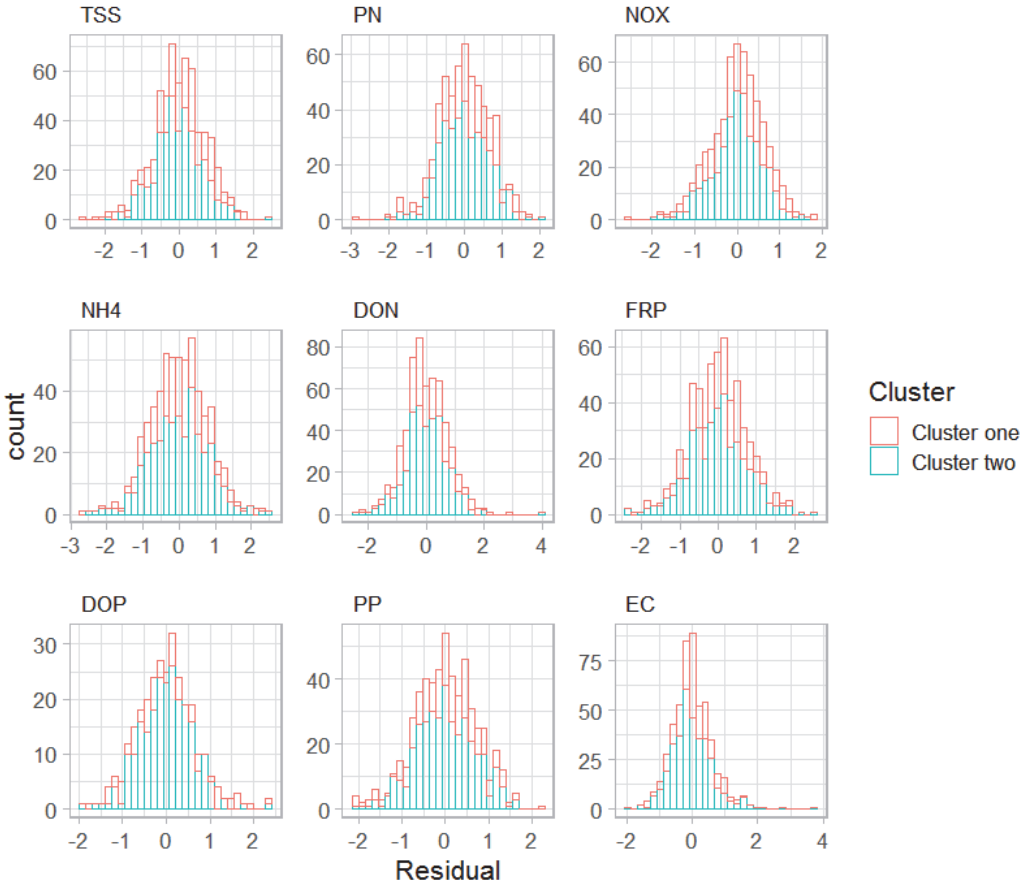

Figure S-35. Histograms showing distribution of residuals of nine constituents from BMA predictions. Red – Cluster one; Blue – Cluster two.

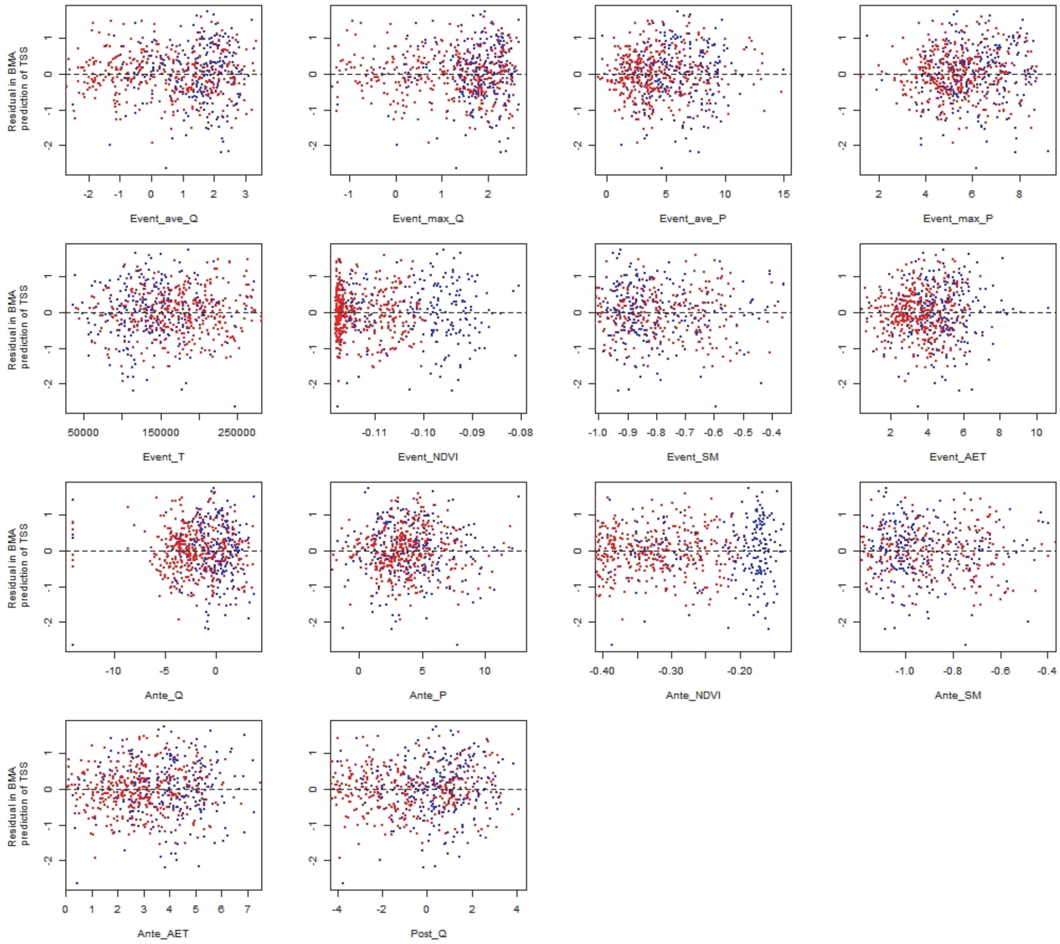

Figure S-36. Relationship between residual in median of BMA prediction of TSS and 14 candidate covariates in BMA. Note, difference colours indicate two clusters: Red – Cluster one; Blue – Cluster two.

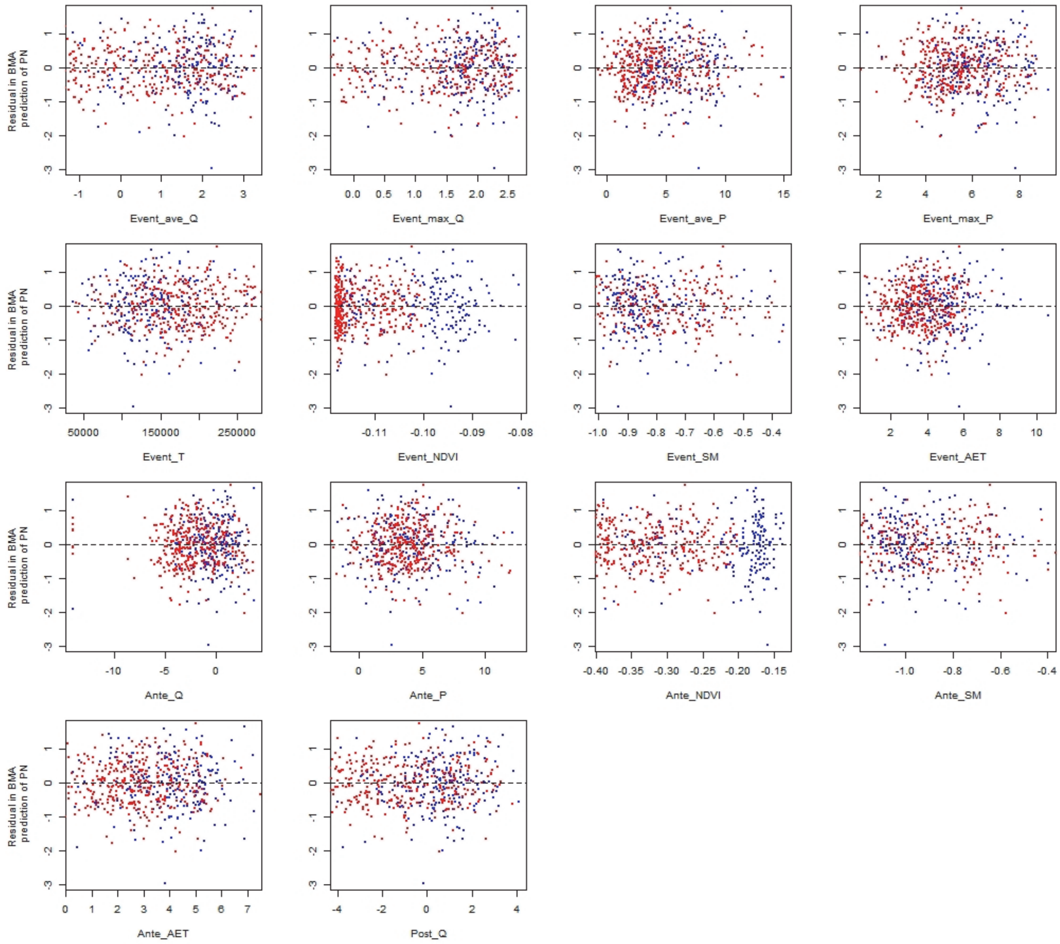

Figure S-37. Relationship between residual in median of BMA prediction of PN and 14 candidate covariates in BMA. Note, difference colours indicate two clusters: Red – Cluster one; Blue – Cluster two.

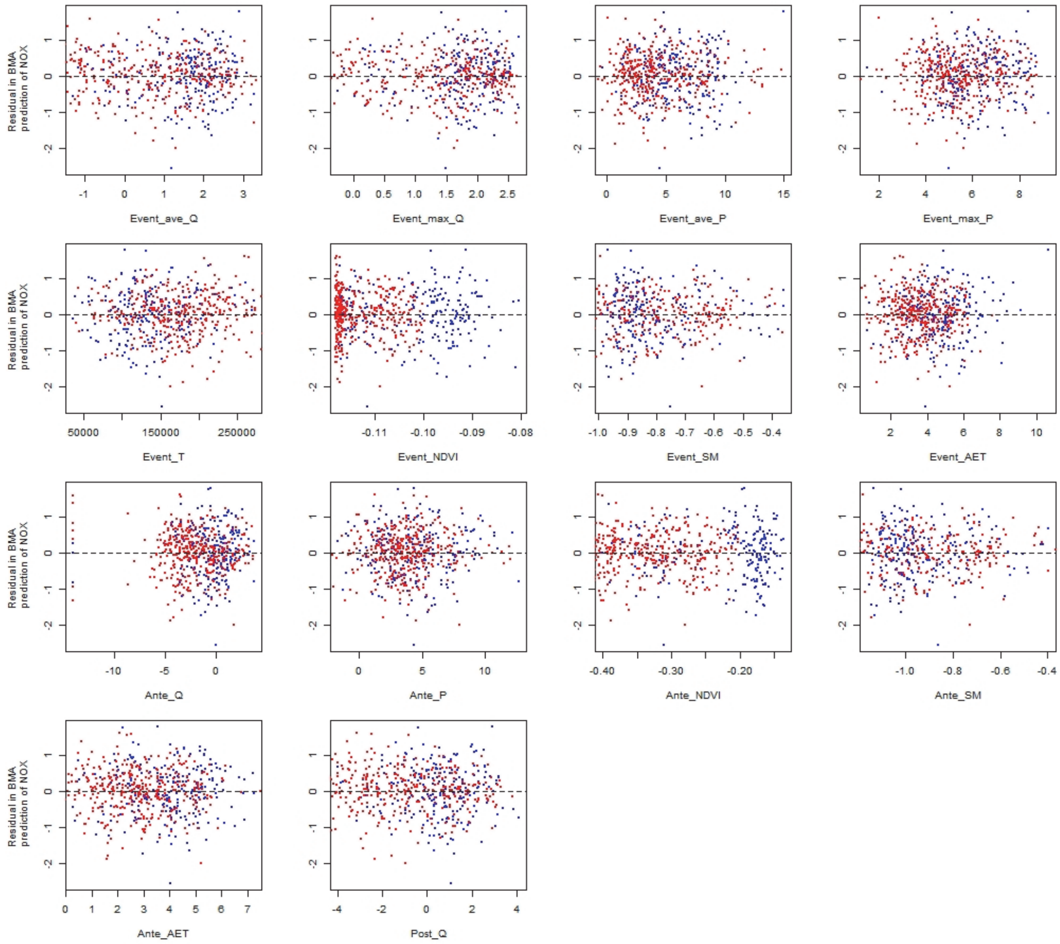

Figure S-38. Relationship between residual in median of BMA prediction of NO_X and 14 candidate covariates in BMA. Note, difference colours indicate two clusters: Red – Cluster one; Blue – Cluster two.

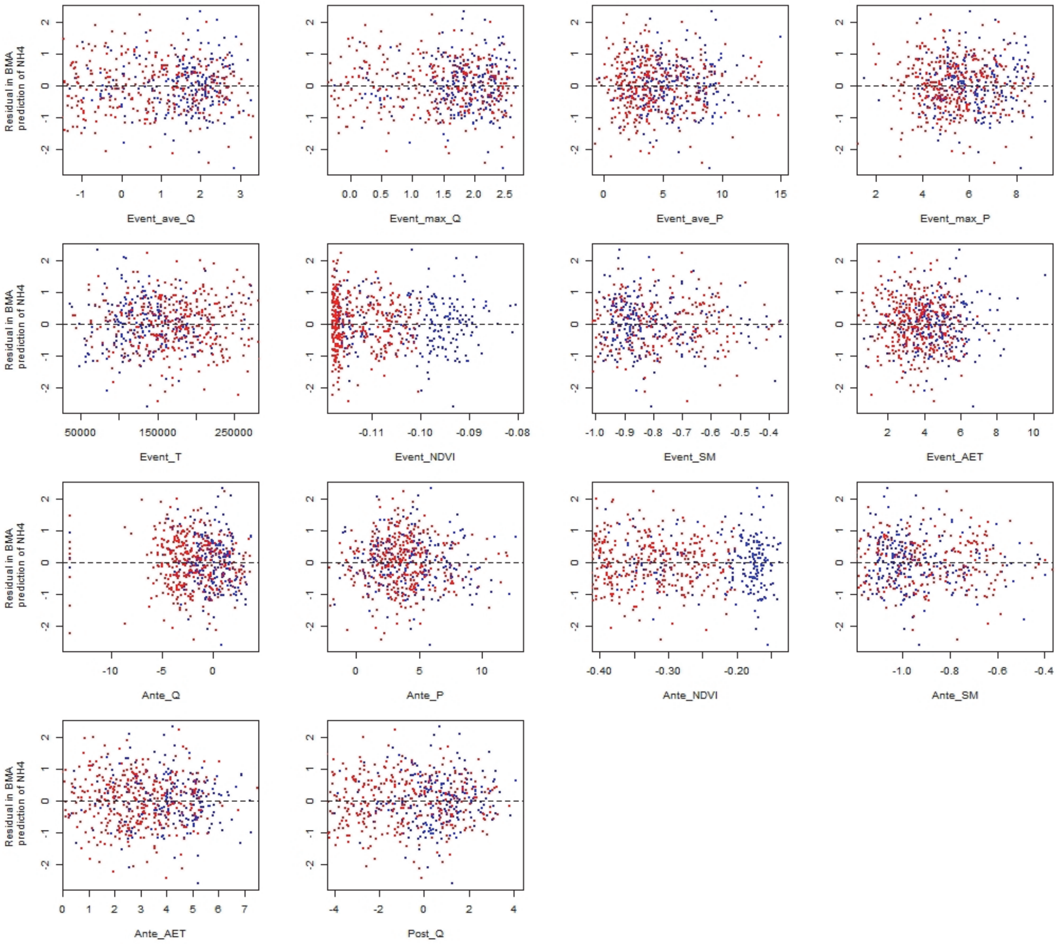

Figure S-39. Relationship between residual in median of BMA prediction of NH_4 and 14 candidate covariates in BMA. Note, difference colours indicate two clusters: Red – Cluster one; Blue – Cluster two.

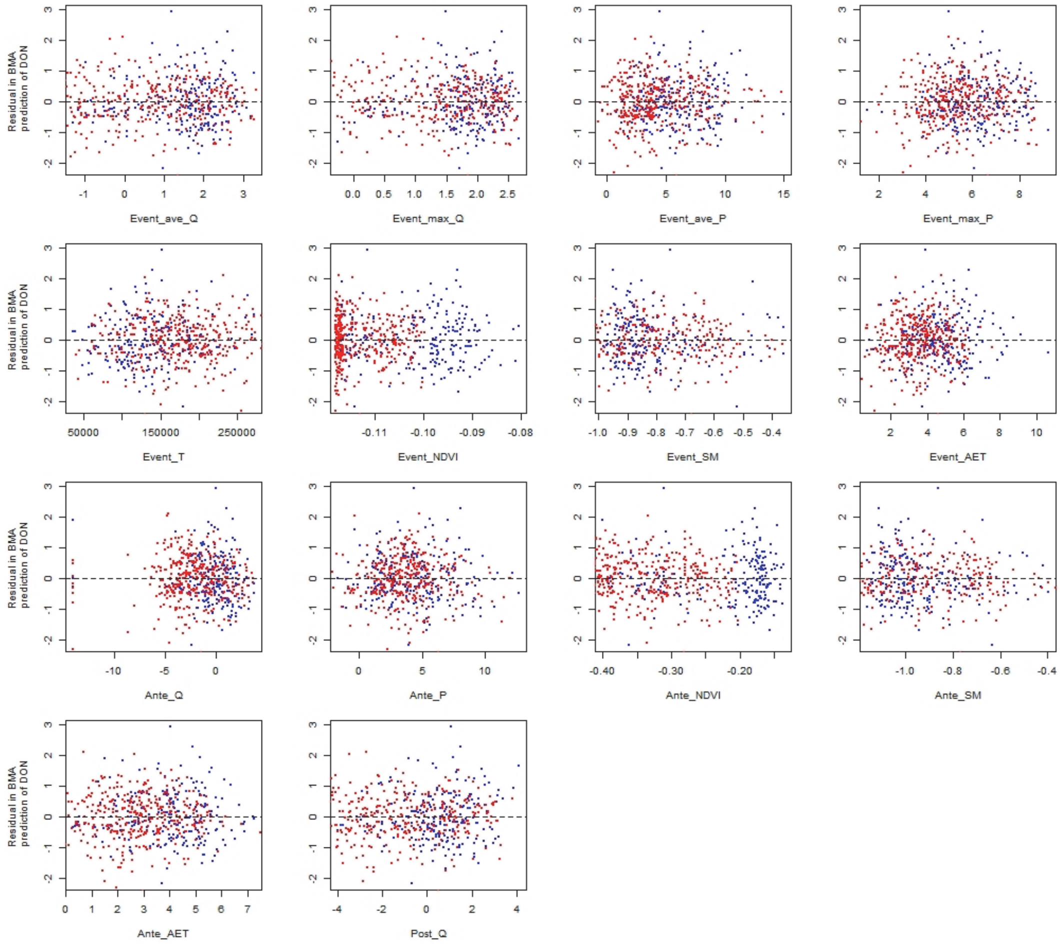

Figure S-40. Relationship between residual in median of BMA prediction of DON and 14 candidate covariates in BMA. Note, difference colours indicate two clusters: Red – Cluster one; Blue – Cluster two.

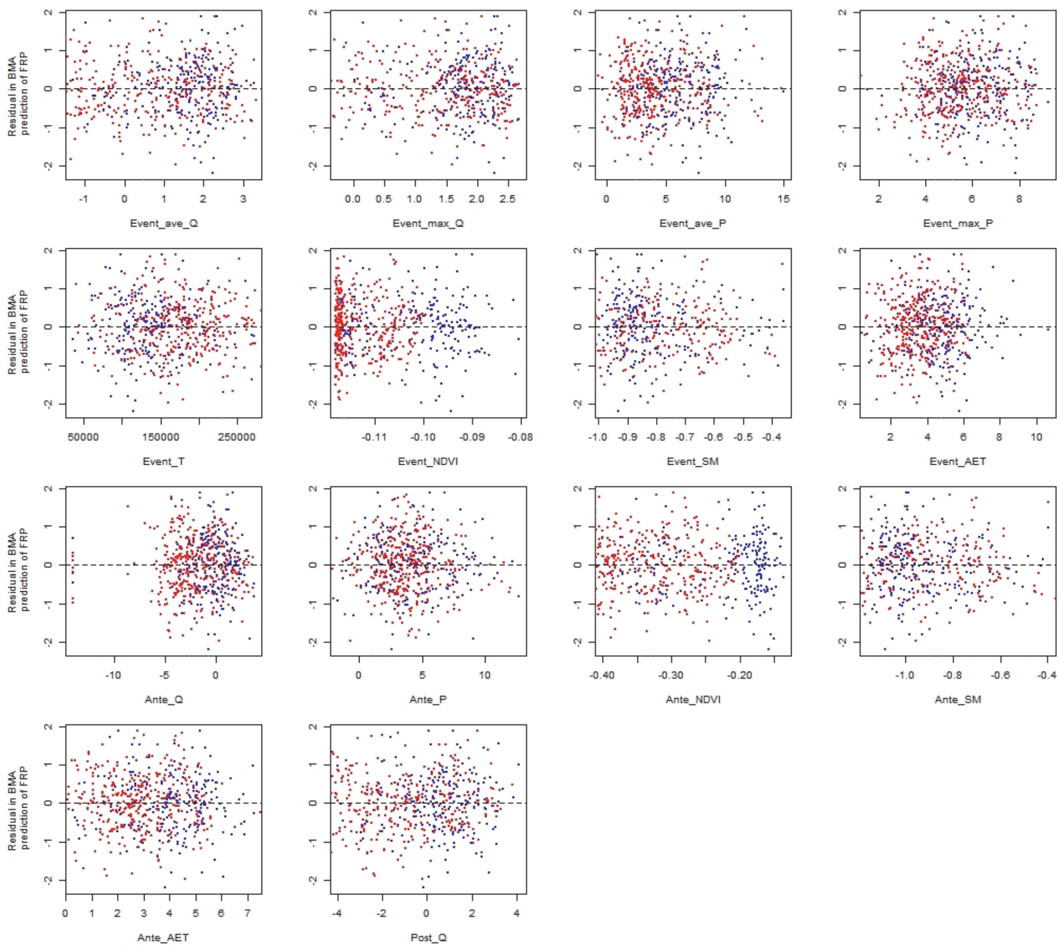

Figure S-41. Relationship between residual in median of BMA prediction of FRP and 14 candidate covariates in BMA. Note, difference colours indicate two clusters: Red – Cluster one; Blue – Cluster two.

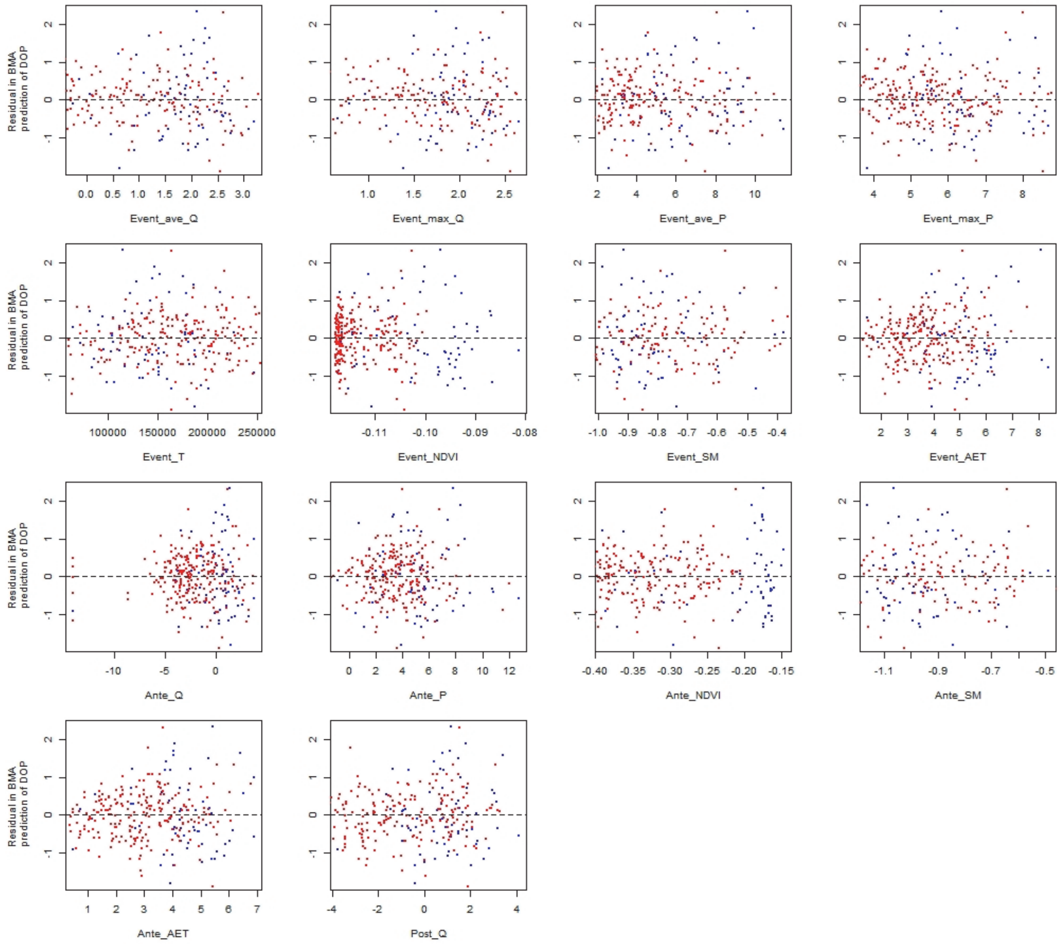

Figure S-42. Relationship between residual in median of BMA prediction of DOP and 14 candidate covariates in BMA. Note, difference colours indicate two clusters: Red – Cluster one; Blue – Cluster two.

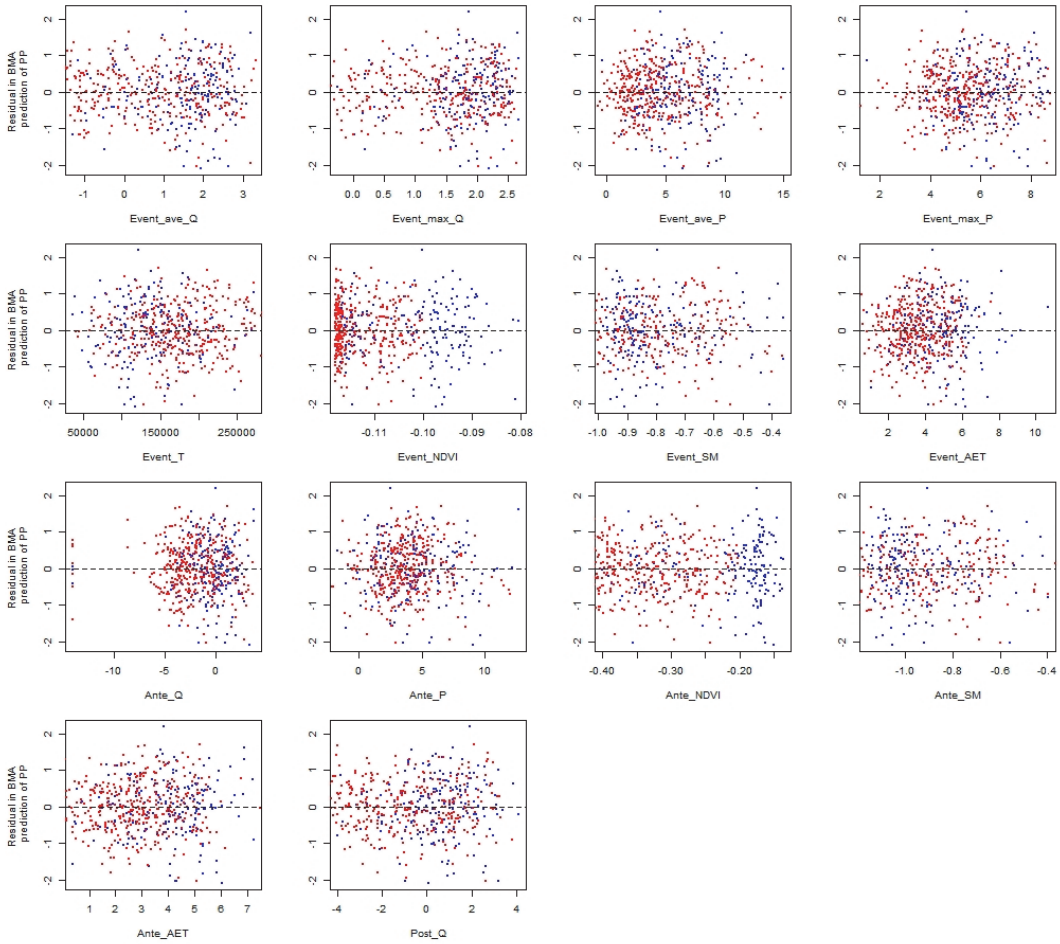

Figure S-43. Relationship between residual in median of BMA prediction of PP and 14 candidate covariates in BMA. Note, difference colours indicate two clusters: Red – Cluster one; Blue – Cluster two.

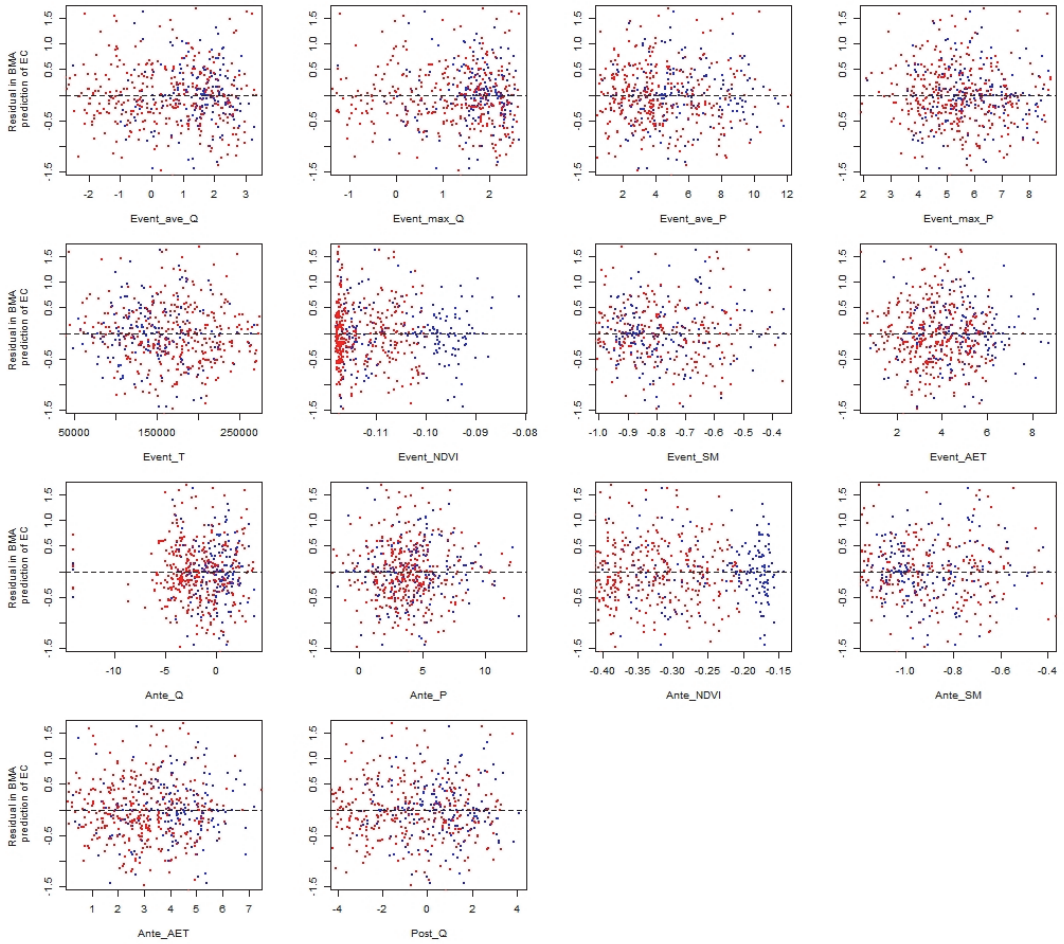

Figure S-44. Relationship between residual in median of BMA prediction of EC and 14 candidate covariates in BMA. Note, difference colours indicate two clusters: Red – Cluster one; Blue – Cluster two.