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Water Management REPORT

FUTURE FOCUSED FRESHWATER ACCOUNTING

Report Appendices

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1 APPENDIX A: INTERNATIONAL CONTEXT

Internationally, there has been increasing momentum in the use and development of environmental accounting in the last two decades. As government, businesses and citizens are increasingly expected to provide evidence that their actions are not unduly degrading the environment and are sustainable and resilient, a range of methodologies in the public and private sectors have been under development and trialled in various contexts. Governments are increasingly expected to monitor and report on their environmental performance, to guide future policy and interventions. There has also been significant investment in developing environmental accounting tools by companies pursuing efficiencies of operation, brand management and sometimes philanthropic considerations.

1.1 United Nations "System of Environmental-Economic Accounting" (SEEA)

This momentum soon generated rapid development of environmental accounting standards and methodological guidance, aiming to achieve coherent, standardised accounting practice to inform environmental reporting, including reporting on water stocks, water flows, and condition and "quality" elements. The most noteworthy of these developments is the System of Environmental-Economic Accounting (SEEA), an international statistical standard developed through the United Nations (UN) and released in 2012. Despite being a rigorous statistical standard insofar as possible, the system was developed to recognise the flexibility needed to accommodate global differences in data availability, environmental and policy needs, etc. Broad consultation with groups trialling earlier efforts to find standardisations for environmental accounts and the balance of rigour and flexibility have led to this being accepted widely as the global standard. Ninety-two countries currently produce accounting reports under this standard and 27 more have them in development. There is also wide uptake by corporations and other non-governmental entities. A variety of SEEA environmental accounts using this standard, including water, are already produced by Stats NZ, along with many other statistical and/or environmental agencies around the world.

Perhaps the most common accounts that people are already somewhat aware of and connect to are the relatively long-standing greenhouse gas (GHG) inventories (accounts) produced by many countries, including New Zealand, under commitments to the United Nations Framework Convention on Climate Change (UNFCCC) and the Kyoto Protocol. These report on anthropogenic emissions and removals of GHGs as a result of energy, industrial processes, agriculture, land use, land-use change and forestry, and waste, following guidelines set by the Intergovernmental Panel on Climate Change (IPCC). Learnings from these inventories, including the need for guidelines, data and methodological support that recognised different countries had differing availability of data, time and the required specialist knowledge were among considerations in the SEEA.

These accounts are relatively mature, having been through several cycles of updating inventories and associated data. Some of what has been learned through this may be relevant to designing New Zealand water and contaminant accounts. With the increasing attention being placed on climate change, there are also likely to be many contexts in which decision makers will wish to place information from the new water and contaminant accounts alongside the greenhouse gas/carbon accounts, as there will be trade-offs and co-benefits at times in decisions that impact the waterways but also GHG emissions.

1.2 SEEA water quantity

The general comments made around developments in the environmental accounting space in the previous section hold particularly true for water. Increasingly the SEEA-Water accounting system is accepted as the international statistical standard, with a conceptual framework and methodological and reporting guidelines for organising water information to study the interaction between economy and the environment. SEEA-Water is a subsystem of SEEA, the internationally accepted international environmental accounting standard, itself designed to be coherent with the long-accepted international accounting standard System of National Accounts (SNA).

After consultation with international experts, SEEA-Water was divided into two parts. Part one includes internationally agreed concepts, definitions, classifications, standard tables and accounts covering the framework, physical and hybrid supply and use tables and asset accounts (Chapters. II-VI). These accepted standards inform many of the quantity focussed questions being asked in this water and contaminant accounting design. However, the sections of the standards most relevant to contaminant accounts (part two), and to potential linkages of the physical/chemical accounts to broader accounts and outcomes, are considered to be "of high policy relevance but still experimental because an internationally accepted best practice did not emerge." It also covers the quality accounts, the economic valuation of water beyond the 2008 SNA and examples of SEEA-Water applications.

The SEEA-Water accounting system can be divided into four components:

1. The physical water supply and use tables, holding information of volumes of water exchanges (flows/fluxes) between the economy and the environment and within the economy.
2. Emission accounts, providing information on amounts of pollutants added to wastewater as a result of economic activities.
3. Hybrid and economic accounts, providing information on the economy of water in monetary terms.
4. Asset accounts, with information on physical stocks of water.

Transboundary flows and methods to report and aggregate/disaggregate data between multiple territories are considered with rigour within the SEEA-Water framework; with examples generally produced for water resources that are shared by several countries, but these are also relevant to transfers between regional authorities or other non-catchment bounded areas we need to produce accounts over. The part of the shared resources which belongs to each riparian country, as well as the origin and destination of specific flows can be explicitly identified. Quota (commitment) information, if agreements to transfer water exist, are part of the reporting standards.

The SEEA-Water Physical Stock Accounts produced by Stats NZ present information on the inflows and outflows of inland water, changes in storage, and some estimates of water use. Along with the methodological approaches used, the data sources, some of which have daily or sub-daily resolutions, and the various data owners indicated in methodological documents underpinning the water accounts, may provide one of the starting sources for generating estimates for the new accounting system requirements being investigated in this document.

Prior to 2021, the accounts were updated with annual data (provided by NIWA and GNS) on an ad hoc basis, with the last release (2018) reporting data from 1995-2014 (https://www.stats.govt.nz/information-releases/environmental-economic-accounts-2018).

Very recently (May 2021), Stats NZ updated the Water Physical Stock Accounts to report up to the end of 2020, and included quarterly along with annual data for the first time (https://www.stats.govt.nz/information-releases/environmental-economic-accounts-water-physical-stocks-year-ended-june-1995-2020).

As these accounts are very newly generated, publicly available information is mostly limited to the core accounting tables and to the NIWA and GNS reports associated with production of the accounts (Griffiths et al. (2021) and GNS Science (2021) respectively). The 2018 release remains pertinent for the purposes of informing our accounting system, as Stats NZ has released a variety of ancillary supporting information, graphical and otherwise, to accompany the core tables and aid interpretation of the results.

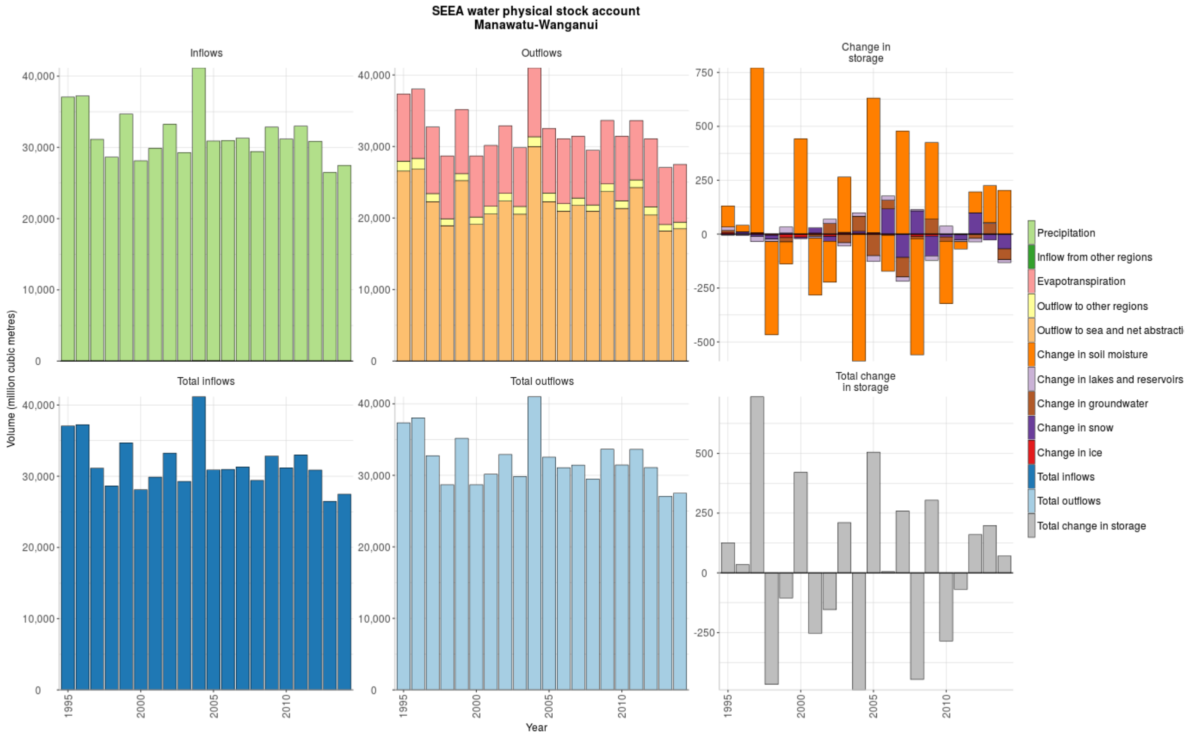

Figure 1: Example graphs from the Stats NZ physical water stock accounts using data from the Manawatu-Wanganui region [https://statisticsnz.shinyapps.io/seea_water_physical_stock] Website accessed and figure downloaded 24/05/2021

1.3 SEEA water quality (Contaminant discharge)

SEEA-Water includes quality accounts since quality is an important characteristic of water and can limit its use. It considers driving forces in terms of the structure of the economy and the population, pressures in terms of the abstraction of water and contaminant discharges into water, and responses in terms of environmental expenditures and the taxes and fees charged for water and sanitation services.

Quality accounts describe the quality of the stocks of water resources. It is difficult, and sometimes not possible, to distinguish changes in quality due to human activities from changes in quality due to natural causes. Although constructing quality accounts may be simple from a conceptual point of view, there are two main issues regarding implementation: the definition and the measurement of water quality classes.

Water quality is generally defined in relation to a specific concern or use; there is little standardisation of concepts and definitions, nor methods for aggregating measurements. Aggregation can be over (a) different pollutants, in order to construct one index which measures the combined impact of pollutants on water resources; (b) single or multiple pollutants in time, in order to address seasonal variations; and (c) single or multiple pollutants in space, in order to reach a single quality measure from multiple measurements at different locations. Quality accounts can also consider reporting on different aspects of a water body. For example, the quality of water running through a river could be reported as very good, even though the riverbed may be reported as severely polluted with heavy metals or other contaminants in its sediment.

In practice, for reporting purposes, quality describes the current state of a particular body of water in terms of certain characteristics, called determinands in the SEEA-Water. The term determinand is used rather than pollutant, parameter or variable in order to underscore the fact that a determinand describes a feature constitutive of the quality of a body of water; it is not exclusively associated with either human activities or natural processes.

Although the SEEA-Water considers water quality accounts, the water quality side of these accounts is in some ways superseded by, but is consistent with, the recently formalised ecosystem condition aspects of the SEEA Ecosystem Accounting (SEEA EA) framework, formally adopted as a statistical standard alongside the SEEA Central Framework (SEEA CF) CF earlier this year.

Ecosystem condition is a key component of the SEEA EA framework (Fig. B.2), defined as *the overall quality of an ecosystem in terms of its main characteristics*. The condition of an ecosystem is expected to be evaluated using quantitative indicators based on good scientific understanding about system behaviour. SEEA EA clearly distinguishes between ecosystem characteristics (i.e. major groups of system properties or components based on ecological understanding), and the metrics that are used to quantify them. *Characteristics* encompass all perspectives taken to describe the long term 'average behaviour' of an ecosystem, including aspects that are insufficiently specific and/or are logistically challenging to measure. These characteristics are estimated using concrete quantitative metrics with precise definitions and measurement instructions. The distinction between characteristics and metrics is essential to operationalise the creation of ecosystem condition accounts. For the selected metrics, SEEA EA notes that accounts should document both the raw variables measured and the generally rescaled and/or aggregated indicators.

Characteristics are represented (b) by variables (c) and indicators (e), where variables have a 'neutral' descriptive function, whereas indicators represent the same information in a normative context (compared to reference levels, (d)). These indicators can be aggregated (f) into relevant sub-indices and indices (g) which synthesize the 'big picture' for policy information.

A condition account includes spatially-referenced condition measures (quality or biophysical) for characteristics such as vegetation, biodiversity (species abundance, diversity indices, rare species), soil, water, carbon air and sometimes, aggregated within governmental or catchment or other boundaries, overall measures (e.g., heterogeneity). Condition is generally summarized in terms of an index. Water quality measures are generally translated into an overall water quality index; other indexes used in SEEA accounting related to water health have considered stream flow rates, capacity to purify water and control floods, and capacity to control erosion (which may be relevant to contaminant accounts in New Zealand).

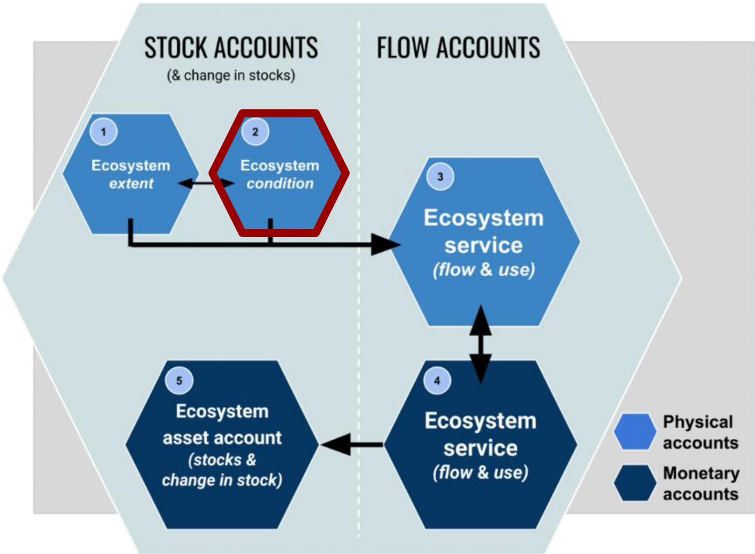

Figure 2: The position of condition accounts in the SEEA EA accounting framework (source: seea.un.org)

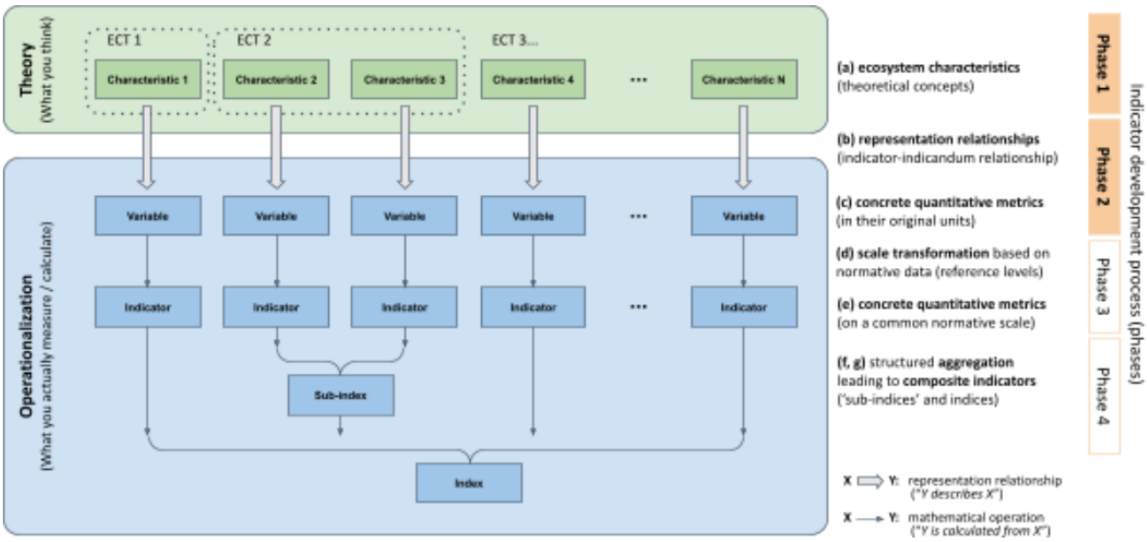

Figure 3: The structure and the main components of an ecosystem condition account for a specific ecosystem type (Keith et al. 2020). Ecosystem characteristics (a) are grouped according to the SEEA ecosystem condition typology (ECT) (Czúcz et al. 2020), which creates a common thematic structure across accounts produced in different countries for different ecosystem types.

1.4 Australia

The Australian National Water Initiative (2004)[1] requires the development of water resource accounting to ensure that '*adequate measurement, monitoring and reporting systems are in place in all jurisdictions, to support public and investor confidence in the amount of water being traded, extracted for consumptive use, and recovered and managed for environmental and other public benefit outcomes*.'

To give effect to this directive, Australian Water Accounting Standards have been adopted as a formal national standard. The purpose of this standard is to guide the preparation and presentation of general-purpose water accounting reports. General purpose water accounting reports are designed to inform users about how water has been sourced, managed, shared, and utilised during a reporting period and to enhance public and investor confidence in the amount of water available, allocated, traded, extracted for consumptive use, and recovered and managed for environmental and other public benefit outcomes.

The objective of general-purpose water accounting reports is to provide report users with information about a water report entity, such as a catchment, which is useful for making and evaluating decisions about the allocation of resources. These decisions may include decisions concerning how water and the rights or other claims to water, will be sourced, managed, shared, and used.

When these reports meet this decision-usefulness objective they will assist report users to evaluate accountability for the management of water resources.

The scope of water accounting in Australia is currently limited to water quantity. Their water quantity accounting systems are relatively mature due to the significant development efforts made by them. In developing their systems, Australia has worked closely with the UN as their respective standards were developed. In essence Australia's water accounting system is the same as the water quantity part of the UN-SEEA.

1.5 Relevance to the New Zealand context

Honouring Te Mana o Te Wai has been a policy commitment in New Zealand since 2014, acknowledging the importance people, communities and institutions increasingly place on both honouring Te Tiriti o Waitangi and recognising the special connection to water we all possess. Te Mana o Te Wai refers to the integrated and holistic wellbeing - health and resilience - of a freshwater body.

Designing a freshwater accounting system to be used as a tool that helps give effect to Te Mana o Te Wai is novel in the context of international water accounting systems, which could be generally argued to treat water as a commodity, a resource to be protected but also exploited. Accounts generated around the world to date are generally concerned with the sustainability of water extraction, provision of ecosystem services, and sometimes consider quality or condition as part of the accounts with a view to protect human use and general ecosystem health. The health of the water bodies for their own intrinsic sakes is not generally considered. The SEEA Water Accounting standard (see SEEA-Water | System of Environmental Economic Accounting) does note Australia and New Zealand as the only two reporting countries that mention the importance of cultural and spiritual values of water along with the more standard emphases on aquatic ecosystem health, and supporting primary industries, recreation and aesthetics, drinking water and industrial use. It also notes that for "the [cultural and spiritual value] categories no quality guidelines are provided".

This provides both opportunity and challenges for New Zealand. We should try to follow international standards where possible, to draw on the many learnings from the international community on trialling accounting over the last decades, but recognise that off the shelf approaches are unlikely to be fully appropriate and that bringing Te Mana o Te Wai fully and appropriately into the design of a freshwater accounting system may be important not just in honouring Te Tiriti o Waitangi but also in informing approaches that may help broader efforts around the world to better recognise intrinsic worth and spiritual and cultural connections to water, forests, key species etc. It is also tempting to take methods from existing systems and work back to find what attributes, characteristics and values could be

[1] https://www.awe.gov.au/water/policy/policy/nwi

reported on but to work from a *Te Ao* Māori perspective arguably means we must make more efforts to find ways to incorporate fundamental values into characteristics and attributes that must be reported on than has been necessary in other jurisdictions setting up experimental water accounting systems.

It is important to recognise that generating water quantity and contaminant accounts will have impacts on people, both those who use them to inform policy or other decisions, and those who are affected by resulting decisions. The accounts must be able to support multiple purposes, strive where possible to be useful and equitable for a range of different stakeholders, and acknowledge that due to this, there may need to be different ways of bringing information out of the accounts. There are different needs and perspectives in different communities, and ways of visualising and presenting the fundamental data and assumptions behind the account may need to be wrapped with different (but consistent) narratives suitable for different (although overlapping) audiences: water users, policy makers, Māori, industry bodies. It is important, therefore, that those responsible for producing freshwater accounts ensure that a broad spectrum of perspectives are represented in the team preparing the accounts.

Acknowledging there are different biases and different needs while respecting and trying to find ways to work together for the common benefit of both people and Te Mana o te Wai may help in securing agreements and resources for actions such as retiring land (for local and/or downstream benefits), co-developing planting for wetland restoration etc.

It is also important to acknowledge that people have financial, social and cultural needs, and that policy or other decisions that are informed by the water and contaminant accounts also need to respect multiple other criteria. Our collective wellbeing is not only influenced by the health and management of our waterways, but by broader ecosystem health, economic drivers and stresses, and social and cultural values inherent in our engagement with land, water and people. The accounts, and the water and contaminants monitored and reported within them, are just one interconnected part of *Kia Whakanuia Te Whenua* (translating along the lines of “People Place Landscape”).

For sustainable land and water management, it has long been acknowledged that social and cultural values and preferences need to be integrated into land-use decision-making along with consideration of environmental and economic goals. Both nationally and internationally, there are efforts and indicators developed and in development that attempt to place quantifications on such values, for use in tracking progress towards goals, among other things. These are generally being developed in line with one or both of the SEEA-Experimental Ecosystem Accounting work and reporting on the UN Sustainable Development Goals (SDG). These goals – a universal call to action to end poverty, protect the planet and “ensure that all people enjoy peace and prosperity” – require countries to report on hundreds of indicators, these being further developed and upgraded as learnings on strengths and weaknesses of current indicators increase. These efforts may help place outcomes from our water and contaminant accounting alongside broader wellbeing and equity measures. It is also important to note that Goal 6 of the SDGs focuses specifically on water, including improving water quality, reducing the proportion of untreated wastewater and increasing recycling and safe reuse of water. Other nationally and internationally relevant concepts developing data and model and reporting standards that may inform or be informed from the New Zealand water and contaminant accounts are advancing in the ecosystem services and similar “natural and social capital concepts”. Both can take an overly human-centric world view, inconsistent with not just Te Ao Māori but broad international concerns about frameworks that can be used to favour valuing nature for instrumental rather than intrinsic reasons. However, for the purposes of designing freshwater accounts, they still hold relevant learnings.

2 APPENDIX B: MEASUREMENT AND MODELLING FOR FRESHWATER ACCOUNTING

2.1 Introduction

This appendix is primarily concerned with providing guidance to users generating accounts on potential data sources and modelling approaches to assist in populating the various components of the water and contaminant stock and flow accounts. Common water and contaminant "IOU" units are discussed and some of the data and models to support associated stock and flow estimates for each unit are explained.

The last section of this appendix provides a more general overview of how modelling approaches fit into and support the accounts. We note although the need for robust data to support the accounts is never questioned, nationally and internationally there have been reservations about the use of hydrological or other models in environmental accounting. Ideally, we would like to have robust measured data at our fingertips to support every element of the accounts, as we arguably have when producing financial accounts (assuming all data on transactions etc. has been properly recorded). However, due to resource constraints, limitations in available measurement techniques, issues in the differing spatial scales (point, plot, census district, catchment, etc) that various data relate to, and our very limited ability to "measure" subsurface stocks and flows, the available spatial-temporal measured data is not in itself adequate to complete the accounts.

2.2 Surface/atmosphere interactions and fluxes

Precipitation and evapotranspiration are fundamental drivers in the hydrological cycle and are listed as line items in the Water Flow accounts.

- Precipitation represents the total flux of water introduced to the land surface, including rain, snow, hail and sleet.
- Evapotranspiration describes the transfer of water from land to the atmosphere by evaporation from soil and other surfaces and by transpiration from plants.
- Potential evapotranspiration (PET) is the evapotranspiration that would occur assuming readily available soil water.
- The actual amount of evapotranspiration (AET) that occurs is equal to or lower than potential evapotranspiration, depending on the amount of water that is available to meet atmospheric evaporative demand.

For accounting purposes, AET should be reported, rather than potential evapotranspiration PET.

When considering the contaminant accounts, an understanding of precipitation and evapotranspiration is necessary along with consideration of additions from and losses to the atmosphere of the contaminant(s) of interest. The Earth's atmosphere is the carrier of a diverse range of trace gases and particles along with its primary constituents (nitrogen (N) and oxygen). Some are emitted by natural sources, others through human activities, and others are the result of chemical reactions within the atmosphere. Contaminants are removed from the atmosphere and deposited onto the Earth's terrestrial and aquatic surfaces through a process known as atmospheric deposition. Contaminants can be deposited by either wet deposition – dissolved or entrained in precipitation – or by dry deposition. Dry deposition includes gravitational settling of particles, or diffusion and turbulent transfer to the surface and subsequent uptake by plants or adsorption to surfaces.

The rates at which atmospheric-derived contaminants are deposited onto the Earth’s land and water surfaces are determined by meteorological factors such as temperature, precipitation, humidity and wind, physical and chemical properties of the contaminant, and surface characteristics where they are deposited.

Plants also actively source certain molecules from the atmosphere, such as carbon. Where N is a contaminant of interest, it is important to note that certain plants have developed strategies to convert atmospheric N to ammonia or related compounds. This conversion is achieved via symbiotic relationships with soil microorganisms, and legumes have a particularly strong symbiosis with N-fixing bacteria. Legumes, particularly clover, have therefore been used for many decades as a mechanism to enhance N levels in New Zealand soils that are naturally low in N. In a study presented by Parfitt et al. (2006), N input and output budgets for the year 2001 were developed for each region and for the whole of New Zealand. Biological N fixation from legumes in pasture was the most important input in almost all regions, excepting Auckland with its large urban population and the West Coast of the South Island, where rainforest significantly out-dominates pasture. Fertiliser application and atmospheric deposition were also significant (the study did not differentiate between N outputs directly linked to fertiliser versus increased stock on pasture and increased urine loss etc). Areas under gorse or other “non-agriculturally productive” vegetation types would also be expected to have high levels of atmospheric nitrogen uptake through fixation.

2.2.1 Measurement

Precipitation, potential evapotranspiration and other climate measurements are routinely made at several hundred gauges across New Zealand (Tait et al. 2006). These stations are operated by NIWA, regional councils and other organisations. Most climate data from these stations is freely available as daily average and/or total from the National Climate Database maintained by NIWA. Note that not all climate measurements are made at all stations, nor have all stations been making measurements without any gaps over time.

For deposition: estimating the deposition of atmospheric pollutants cannot be measured as simply as many other atmospheric variables. Field measurements of atmospheric pollutant concentrations are made both in ambient air and dissolved in water and combined with modelled estimates of deposition velocities derived from aerosol physics principles.

For fixation: methods will vary depending on the contaminant of interest. For N, the most popular measurement technique to determine the N fixation rate is the acetylene reduction assay method, using gas chromatography. Where N is assumed to be the main limitation on growth, simpler methods assuming correlation between dry matter yield and N uptake can be applied, with other N sources available to the plant assessed.

2.2.2 Modelling

Two types of modelled climate products are highly relevant for producing IOU water accounts. First, interpolation models provide spatial infilling of the precipitation and evapotranspiration measurements made at individual climate stations. These interpolations can be used to assess conditions at the time of measurement, and also for hindcasting purposes based on previous measurements. Second, numerical weather prediction models provide estimates of precipitation and evapotranspiration in the future. These prediction models operate over different time horizons: near-term (ca. 48-72 hours), seasonal, or longer-term (multi-decadal).

Interpolation of the measured climate data at the national scale, over a regular (~5 km) grid, is provided by the Virtual Climate Station Network (VCSN) operated by NIWA. The VCSN provides estimates of daily rainfall and other climate variables such as air and vapour pressure, maximum and minimum air temperature, soil temperature, relative humidity, solar radiation, wind speed at each grid point, and data derived from them, such as potential evapotranspiration and soil moisture. The climate data estimates are produced every day, based on a spline interpolation of the actual measurements made at climate stations located around the country (Tait et al. 2006). For each site, selected percentiles in the historical measurements are also provided to assist with uncertainty evaluation (Figure 4).

Wide-scale estimation of AET over bare and vegetated land generally requires measured or modelled soil moisture estimates along with potential evapotranspiration, and a function reducing the fraction of PET that is actually evaporated as soil moisture levels drop below critical points (such approaches are referred to as soil moisture accounting). Most catchment scale flow models take PET along with precipitation as input driving data, and internally calculate and report back estimates of actual evapotranspiration and soil moisture through some form of soil moisture accounting.

Interpolations of measured climate data may be available at higher spatial and/or temporal resolution for some parts of the New Zealand.

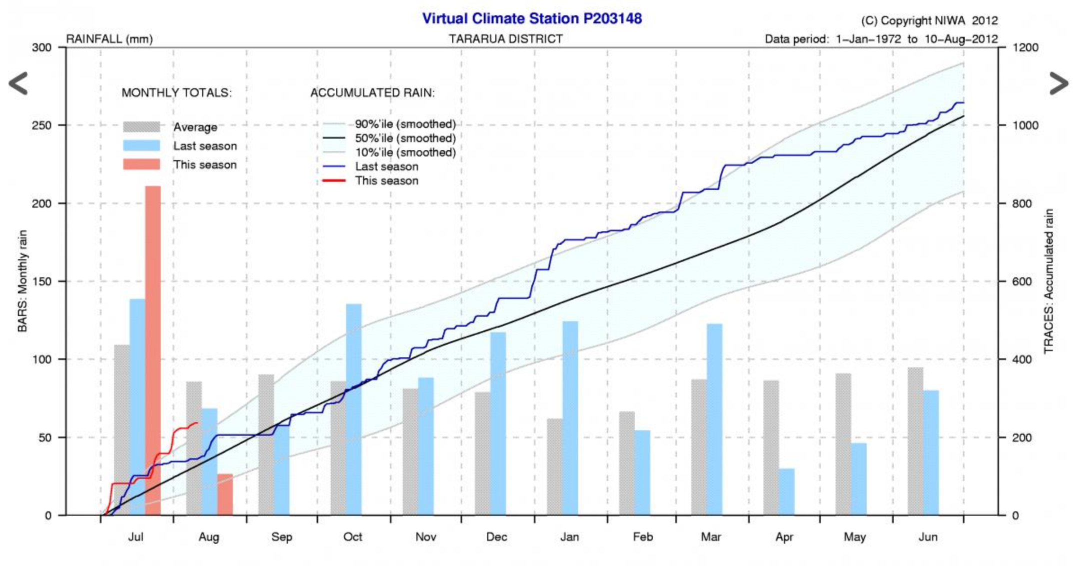

Figure 4: Example VCSN daily rainfall accumulation plot for a site near Dannevirke, Tararua District. Source: www.niwa.co.nz/climate/our-services/virtual-climate-stations.

Short-term forecasts for precipitation and evapotranspiration, along with other climate variables, are available from current national-scale numerical weather prediction models. The New Zealand Limited Area Model (NZLAM) operated by NIWA is a national-scale numerical weather prediction model based on the UK Met Office Unified Model. NZLAM provides weather forecasts out to 72 hours ahead; the forecasts are generated four times daily for a horizontal grid resolution of about 4.4km. NIWA also operates the higher-resolution New Zealand Convective Scale Model (NZCSM). NZCSM uses initial conditions interpolated from NZLAM onto a 1.5km grid and produces forecasts out to 48 hours ahead, generated four times daily.

Seasonal climate outlooks[2] look further forward in time. These seasonal climate outlooks are produced quarterly based on models that account for drivers such as the Southern Annular Mode and the El Niño Southern Oscillation. The spatial resolution is roughly regional and measures of the confidence are provided, which can assist with incorporation of uncertainty into water accounting forecasts (Figure 5).

[2] https://niwa.co.nz/climate/seasonal-climate-outlook

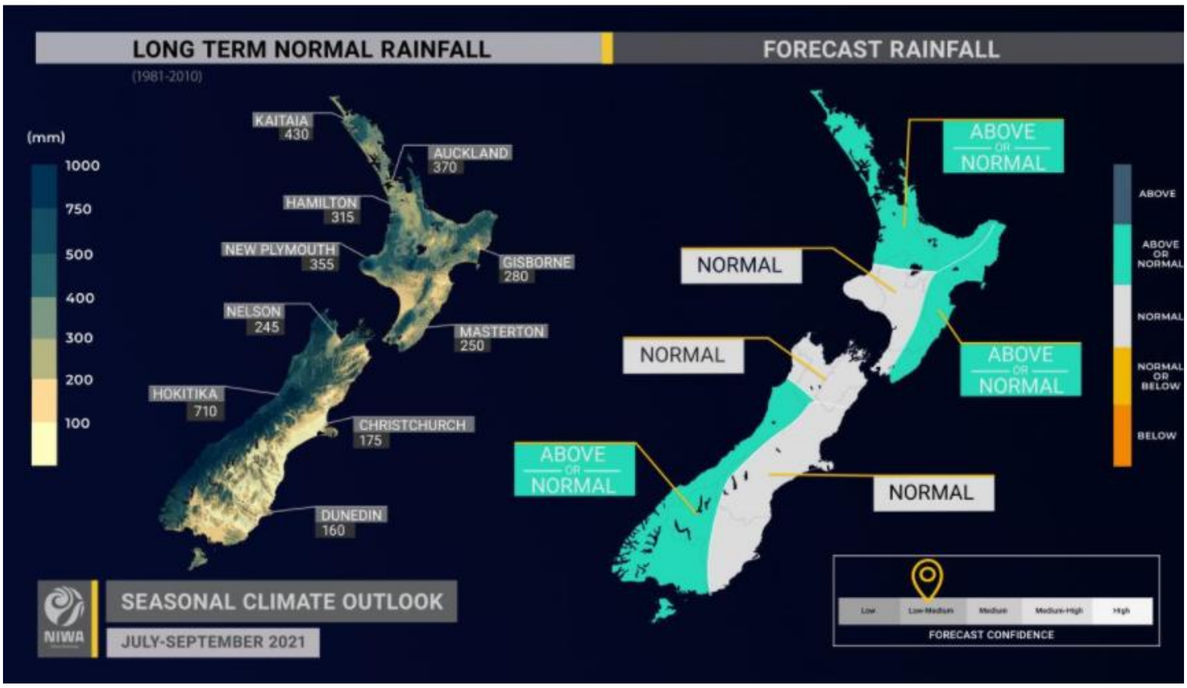

Figure 5: Example rainfall forecast map from seasonal climate outlook, covering the period July to September 2021. Source: www.niwa.co.nz/climate/seasonal-climate-outlook.

Longer-range climate projections have also been produced for the years 2040, 2090 and 2110 at the national scale (Ministry for the Environment 2016). These climate projections are based on Global Circulation Models that have been downscaled and validated for New Zealand. The projections are calculated for a set of representative concentration pathways (RCPs) defined in the 5th assessment report of the Intergovernmental Panel on Climate Change (IPCC), where each RCP describes a possible scenario of greenhouse gases released into the atmosphere globally and through time (Figure 6). The spatial resolution is sub-regional and projection uncertainty is quantified by comparing outputs of over 20 individual models included in the ensemble.

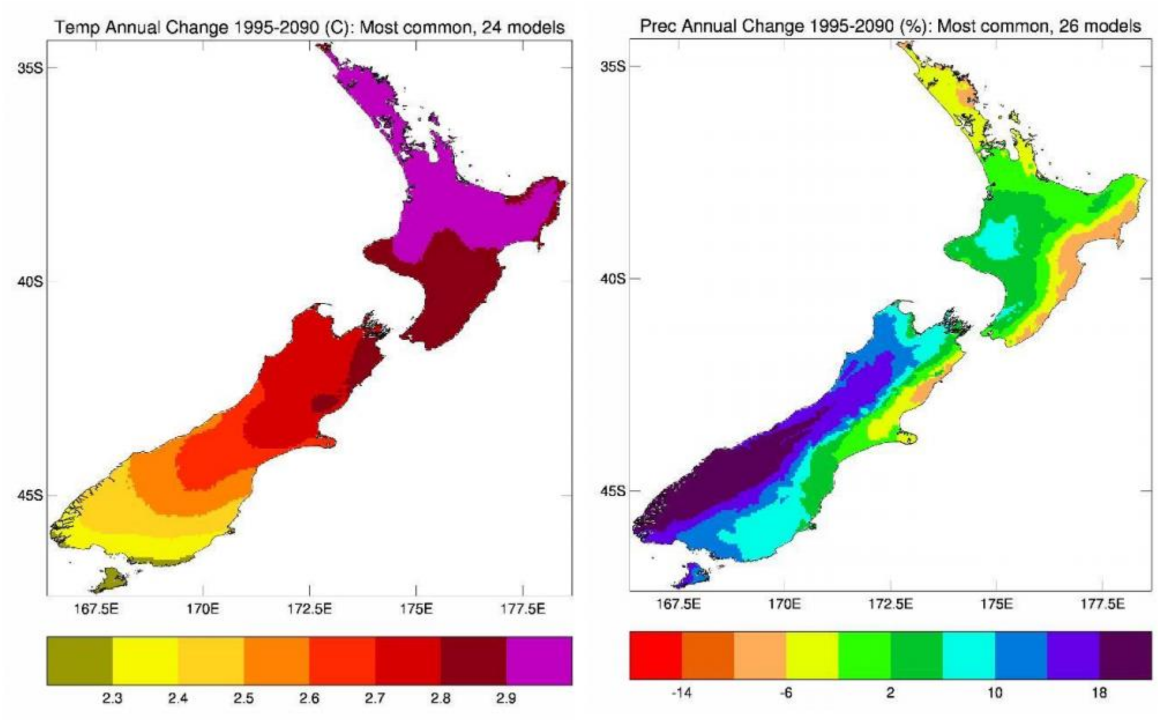

Figure 6: The most common patterns of projected change in annual temperature (left) and precipitation (right) between 1995 and 2090 under a high-emissions scenario (RCP8.5), based on ensemble averages from statistical downscaling results of 24 and 26 GCMs, respectively. Source: (Ministry for the Environment 2016).

For deposition: point source "measurements", which already include some modelling through the use of the aerosol physics equations of motion, then need to be combined with some forms of interpolation and perhaps supervised machine learning to produce maps of deposition for different atmospheric pollutants.

For fixation: the gas chromatography method is a relatively direct measurement, but some modelling, or at least assumptions of correlation are made if using estimation methods based on assuming proportionality between N availability and plant growth. Otherwise, there is little further modelling on the fixation itself, but fixation estimates do go on to inform general modelling tracking contaminants through soils, groundwater, rivers, lakes, etc.

2.3 Soils

For the purpose of this report, soils are considered to be that part of the subsurface contained in the biologically active soil zone. Soil moisture and soil contaminants are accordingly referenced as that water and contaminant mass held in that biologically active zone; the deeper unsaturated and saturated groundwater zones are discussed in the groundwater section.

The transport and potential transformations and/or decay of contaminants within soil are non-trivial to measure and predict, due to their chemical, physical and biological complexity and spatio-temporal variations. Soils, and the vegetation and microorganisms within soils, play a key role in moderating the exchange of water and chemicals between the atmosphere, deeper subsurface and water bodies. The mass of a given contaminant will be the sum of that present in dissolved form, that attached to or within the soil matrix surface (sorbed) and that present in gaseous form in soil pore spaces. Considering the physical movement of contaminants, chemicals can be transported dissolved in water, as particulate matter entrained in water flowing through large pores, as particulates attached to soil moving through geomorphic processes (e.g. erosion, landslides), or via volatilisation back to the atmosphere.

Certain contaminants are either primarily dissolved or primarily in solid form/sorbed, in which case their transport mechanisms are primarily through soil water flow alone or direct movement of soil alone respectively, Others are more “in-between” – they may travel for a distance in dissolved form, become lodged onto the soil matrix partway, and eventually again become dislodged and continue travelling in dissolved form. This process can be very random at the individual particle level, but when large numbers of particles are involved, the overall effect is a retardation of the time a fully dissolved particle would take to transit through the soil. Although there are general guidelines as to the proportions of chemicals likely to be dissolved versus in particulate form, these can change depending on soil make-up and other environmental conditions such as temperature and pH. Bioavailability of the contaminant is also important in understanding potential biotic uptake and transformations, and chemical transformations and sometimes decay processes also need to be considered.

Ignoring biogeochemical transformations and decay, which must be considered separately for each contaminant, chemicals travelling within water are primarily subject to advection – moving with the bulk flow of water; diffusion – the movement of chemicals from high concentration to low concentration, and mechanical dispersion – a smoothing effect similar to diffusion caused by individual particles talking a variety of routes through soil or other porous mediums – some slower, some faster than the average bulk rate of advection.

2.3.1 Measurement

Soil moisture at 100mm depth is estimated at some of the several hundred meteorological monitoring gauges across New Zealand (Tait et al. 2006). These stations are operated by NIWA, regional councils and other organisations. In addition there are a few thousand soil moisture sensor sites operating on farms throughout New Zealand. Most of these sites are on irrigated farms. Soil moisture, and more general soil properties, are highly variable spatially (including variability in depth along with x-y lateral variations). The spatial density of soil moisture sensors is too low to provide a robust estimate of the volume of soil water stored in a catchment or sub-catchment at any particular point in time. Point source (sensor provided) soil moisture data is probably best used in conjunction with satellite data and models to estimate soil water stocks and flows.

The measurement of contaminant losses from soils to groundwater and/or open water bodies has been routinely done by scientists trying to assess how losses vary from different land use or land use practices. Additional data on losses have been collected as part of regulatory compliance by Regional Councils (including unitary authorities), or for educational purposes by community, industry, or Regional Council groups. Despite these efforts, the great variability in soils, management, climatic conditions, vegetation etc. means there is still very limited data available to support decision making and model parameterisation purposes, particularly for less-studied soils and vegetation / crop types.

For diffuse sources of contamination in rural areas, a variety of methods are available to assess surface and near surface flow paths (overland flow and flow from soils directly to waterways) or deeper sub-surface (leaching) flow paths. These flow paths are normally assessed at a small scale and designed to measure the land use or land use practices accurately avoiding error or attenuation caused by changes occurring in-stream or within the soil zone. The methods are designed to capture a representative, and known, volume of flow and allow for their contaminant concentrations to be measured. The product of flow and concentration is used to establish a load of contaminant lost, which is often adjusted to an area-specific annual yield that can be used to assess relative changes in land use or land use practices. Yields are often termed export coefficient, especially in urban settings (Gadd et al. 2018).

A full review of the advantages and disadvantages of each method is beyond the scope of this document, but can be found elsewhere (Weihermüller et al. 2006). Briefly, for measuring subsurface flow, methods in common use in New Zealand include: barrel and channel lysimeters that, respectively, encase intact soil monoliths (Cameron KC et al. 1992) or intercept subsurface flow from above via a pan inserted horizontally into the soil (Carrick et al. 2011); methods that utilise capillary action (Norris et al. 2017) to draw (wick) drainage from an intact soil with or without a casing or active suction via a cup and probe or tension plate inserted into the soil (Curley et al. 2011); and methods that measure contaminants in a soil extract (McDowell R and Condron 2004) or use exchange resins to capture contaminants (Jarvie et al. 2008). Methods for measuring surface flows include weirs and flumes that are twinned with automatic samplers to sample intermittently or continuously flowing small streams (Smith and Owens 2014) and runoff boxes than bound topsoil field plots and collect surface runoff at a downslope outlet in response to surface runoff events (McDowell Richard W and Norris 2014).

2.3.2 Modelling

Due to the limited number of point observation sites and the sensitivity of soil moisture responses to non-meteorological factors such as soil type, vegetation and topography, estimating soil moisture over space through interpolation methods is risky, and "soil moisture accounting" approaches are more normally used, either stand-alone or embedded within more complex hydrological catchment models. Reasonable estimates of soil moisture are also important to allow reasonably accurate estimation of actual evapotranspiration, which depends on both precipitation and soil moisture as previously mentioned in the precipitation and evapotranspiration section.

In stand-alone methods, a simple "soil bucket" approach can be used where important thresholds based on soil type and vegetation type are set to understand when moisture and rainfall inputs are such that drainage occurs (when field capacity is exceeded) and/or overland flow (when the soil reaches saturation), and when the soil moisture drops to a level where plants become water stressed and actual evapotranspiration reduces below potential evapotranspiration rates. Many irrigation scheduling models use some form of this approach, e.g. IrriCalc and SPASMO.

Most catchment scale flow models embed approaches along these lines also, sometimes with further detail on topographical influences and other factors (e.g. TOPNET, LUCI), and internally calculate and report back modelled estimates of actual evapotranspiration, soil moisture and drainage from soils to deeper groundwater along with estimates of overall water delivery to rivers, lakes, etc. In many accounting contexts it should be possible to choose a model or integrated modelling system that supports soil moisture content and flow calculations along with the river, groundwater recharge and evaporation calculations. Models are used to augment or supplement the measurement of contaminant concentrations or loads. At the land-water interface scale, the term 'model' can encapsulate tools that range from simple risk indices and calculators to complex process- or mechanistic-based models.

Table 1 gives an account of the key characteristics for some models in common use in New Zealand that could be used in freshwater accounting at the land-water interface. Freshwater accounting using risk indices has been used overseas where risk is scored relative to, for example, a load of nutrient loss at a field or farm scale. Such risk-loading relationships are recognised in plans by regional councils as part of Farm Environment Plans (FEPs) and driving actions in the implementation of FEPs to achieve catchment outcomes. In addition to the models listed in Table 1, other models of the land-water interface are available overseas. However, these were not included owing to a much larger gap in capability and capacity and in available data to use them. These overseas models would require substantial effort to calibrate them for local conditions. Such models include, but are not limited to: Annual phosphorus Loss Estimator (APLE) (Vadas et al. 2015); Agricultural Policy Extender (APEX) (Mason et al. 2020); Dairy Forage System Model (DAFOSYM) (Rotz C et al. 1989); Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) (Leonard et al. 1987); Integrated Farm Systems Model (IFSM) (Rotz A 2018); Nitrate Leaching and Economic Analysis Package (NLEAP) (Shaffer et al. 1991).

Table 1: Key characteristics of models commonly used in New Zealand to estimate contaminant leaching to meet current regulatory requirements.

Model	Spatial scale	Temporal scale	Quantification	Use in regulation	Reference
APSIM	Point, but scalable to block or farm	Daily to annual	N load	Used in farm and catchment modelling by at least one regional council	Holzworth et al. (2018)
Beef and lamb FEP	Block to farm	Annual	Risk of N, P and sediment losses	Used for FEPs in the sheep and beef sector	Beef and Lamb NZ (2019)
CadBal	Point, but scalable to block or farm	Annual	Cadmium load	Used by the fertiliser industry and Ministry for Primary Industries to ascertain compliance with voluntary Cd limits in P fertiliser	Gray & Cavanagh (2020)
DairyNZ	Farm	Annual	Reductions in N, P, sediment, and *E. coli* losses from practices as a risk relative to nearest water quality monitoring site	At beta phase, still in development	
Deer Industry Environmental Code of Practice	Farm	Annual	Identifies but does not quantify relative risk of practices for N, P, sediment, and *E. coli* losses.	Used to inform FEPs for deer farmers	Deer Industry NZ (2018)
Fonterra risk index	Field to farm		Risk of N, P, sediment, and *E. coli* losses from practices as a risk	Used for FEPs for Fonterra suppliers	Fonterra (2020)
MitAgator	Point to farm	Annual	Load and load reductions N, P, sediment, and *E. coli* losses from practices	Used for FEPs	McDowell et al. (2015)
OVERSEER	Block to farm	Annual	Load of N and P	Used in farm and catchment modelling by many regional councils	Overseer (2016)
SPASMO	Point, but scalable to block or farm	Daily to annual	Load of N and P	Used in farm and catchment modelling by at least one regional council	Sarmah et al., (2005)

2.4 Groundwater

For the purpose of this report, groundwater is defined as all water below the ground surface in the unsaturated (vadose) and saturated zones but excluding soil moisture in the biologically active soil zone discussed in the soil section. Depending on the geographical context, geothermal water could be included in freshwater accounts as groundwater, or as a transfer into groundwater (or surface water) from an external source of water and contaminants.

New Zealand's groundwater is contained within approximately 200 aquifers (Figure 7). The total national stock of groundwater that contributes to river baseflow has been estimated to be 1392 km^2, with an additional 265 km^2 of deeper groundwater that is assumed to be largely hydraulically isolated from surface water (Toebes 1972). However, as for lakes (see Section 2.6), due to the challenge of accurately determining the total volume of groundwater in New Zealand's aquifers, the national accounts presently only report on the relative change in groundwater stocks.

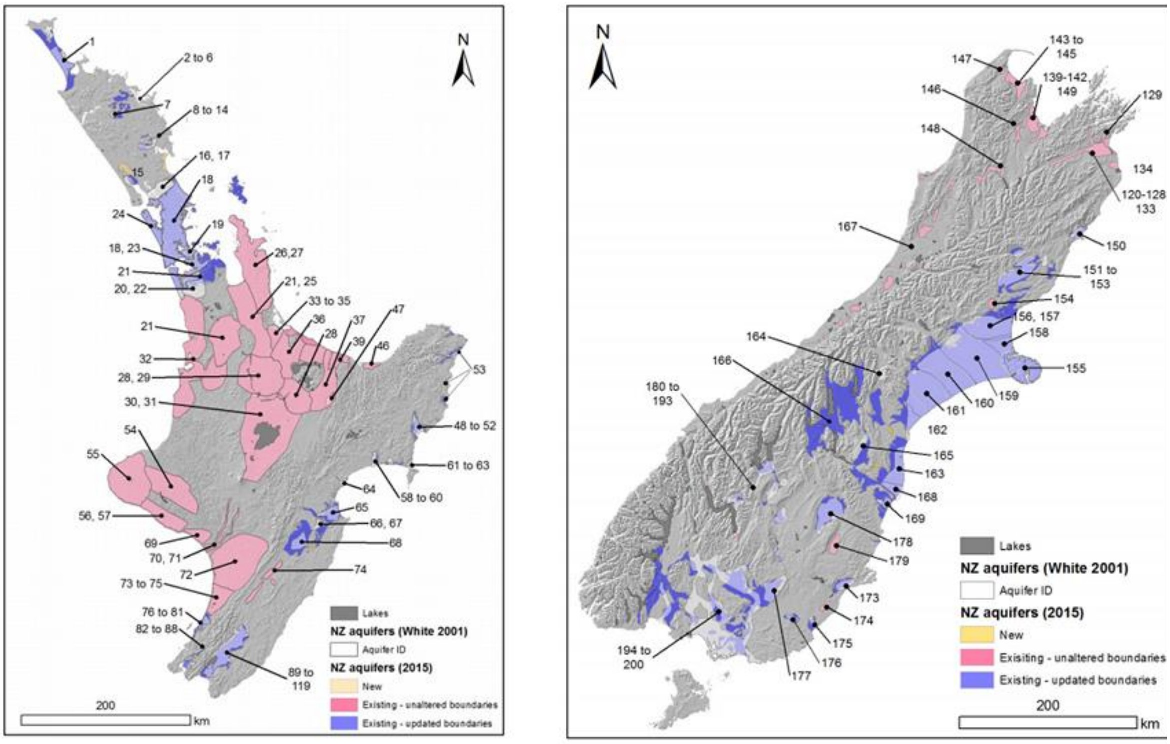

Figure 7: Locations of New Zealand aquifers as originally mapped in 2001 (White P 2001) and subsequently updated by in 2015 (Moreau M and Bekele 2015). Source: (Moreau M 2020)

In addition to discussion of total and relative changes in groundwater stocks overall, this section also discusses exchange flows of groundwater into/out of rivers, lakes and wetlands, and inflows to groundwater soil and outflows of groundwater to the sea.

2.4.1 Measurement

2.4.1.1 Inflows

Recharge is the process by which water enters the subsurface, either via seepage of precipitation or irrigation return flows through the soil zone (Land Surface Recharge, or LSR), or via seepage from surface water bodies such as rivers, lakes or wetlands (Surface Water Recharge, or SWR).

Measurement of LSR is undertaken using lysimeters of various types as reported in various New Zealand studies (e.g. White PA et al. (2013); Duncan et al. (2016) and guidelines (Lovett 2015). These lysimeter measurement methods typically involve capture of drainage water beneath an encased intact soil column using a tipping bucket gauge (refer to Section 2.3.1 on contaminant losses from land). Two to three such lysimeters are often paired at each site to enable comparison of measurements. Normally, local measurements of precipitation, evapotranspiration, irrigation etc are made so that the observed lysimeter drainage volumes can be expressed in the form of proportion of rainfall or irrigation return flow. There are presently approximately 25 recharge lysimeters in operational farms across five regions of New Zealand, each providing localised measurements of LSR in their immediate vicinity (Figure 8).

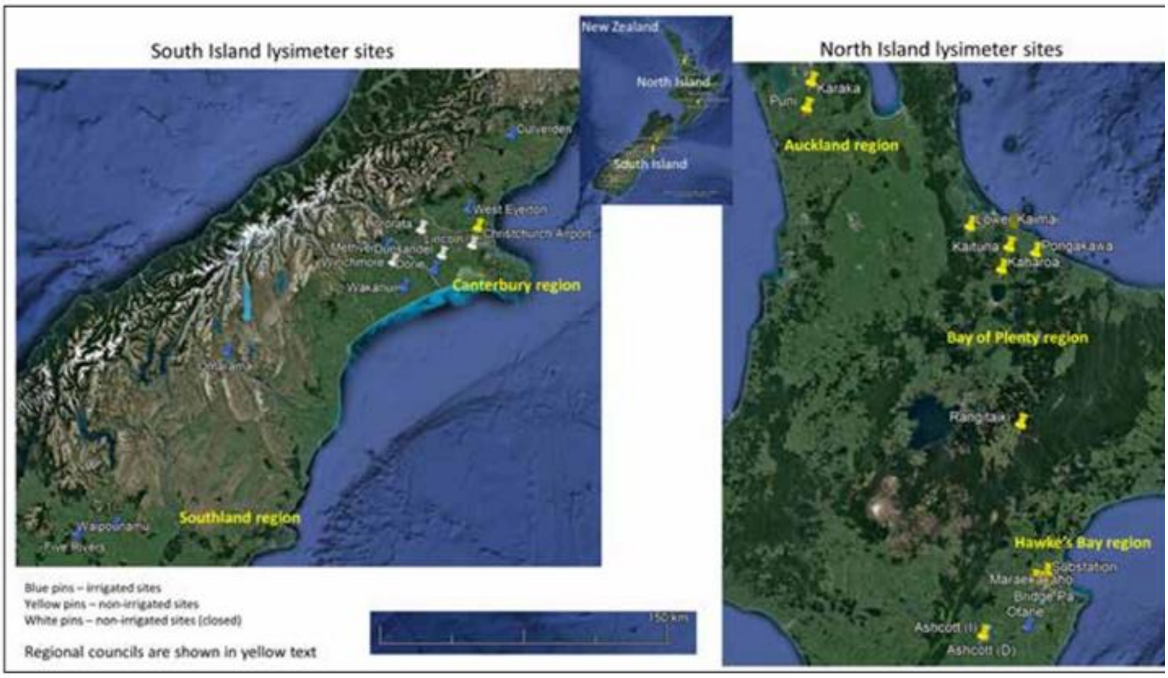

Figure 8: Distribution of recharge monitoring lysimeter sites in New Zealand as of January 2019. Source: (Srinivasan and Lovett 2019).

Direct measurement of SWR from rivers is most commonly undertaken via concurrent flow gaugings, whereby the flow in the river channel is measured upstream and downstream of the losing reach and the difference is attributed to SWR (Cameron S and White 2004; Baalousha HM 2012a). Measurements of vertical gradients in groundwater level and/or groundwater temperature have also been used to infer SWR (Coluccio and Morgan 2019), though these methods are less commonly employed in New Zealand.

2.4.1.2 Internal flows

Groundwater flow velocity within the aquifer can be directly measured in situ with a variety of types of devices suitable for installation into individual wells (Bayless et al. 2011). One common type of groundwater velocity probe measures the travel time of a conductive tracer injected on one side of the probe and detected on the other (Labaky et al. 2009). This type of velocity probe has been tested in New Zealand, though its use is not widespread (Zemansky G and Devlin 2013). Other types of groundwater velocity probes measure the transport of temperature pulses or use optical sensors to track the motion of suspended colloids (Bayless et al. 2011). In addition to such probes, groundwater velocity can also be estimated by timing the rate of dilution of a tracer (e.g. salt) added to a well (Labaky et al. 2009). Aside from these single-well methods, groundwater velocity can also be measured using inter-well techniques, normally by injecting a non-reactive tracer such as a chemical, isotope, colloid or heat into one well and timing its appearance in another down-gradient well (Devlin 2020). Note that all of these single- and inter-well methods for measuring flow velocity provide only very localised measurements immediately around or between the well(s), which can be useful for fine-scale investigations but can be challenging to upscale for application at the larger scale common to many groundwater studies. At the larger scale, groundwater flows can be estimated through the use of age tracers such as tritium, chlorofluorocarbons and sulphur hexafluoride (Stewart and Morgenstern 2001); however, interpretation of groundwater flow rates from age tracer measurements required some form of modelling and therefore is discussed in the Modelling subsection below.

2.4.1.3 Outflows

Discharge is the process by which groundwater exits the subsurface. Groundwater discharge can occur into parts of some rivers, lakes and/or wetlands, and/or into the sea (for coastal aquifer systems). Abstraction of groundwater e.g. for irrigation, bulk water supply, etc. is also considered a form of discharge for water accounting purposes but is discussed in Section 2.10.

Groundwater discharge into rivers is most commonly measured using concurrent gauging surveys: as noted above, a reduction in flow between upstream and downstream gaugings indicates loss SWR, whereas an increase in flow would indicate groundwater discharge into the river (see also Cameron S and White (2004), Baalousha HM (2012a)). Complementary with concurrent gaugings, groundwater discharge into a river reach can also be evaluated using radon mass balance (Martindale Heather et al. 2016; Morgenstern et al. 2018) or vertical/longitudinal temperature profiling (Donath et al. 2015; Moridnejad et al. 2020), though these methods are less commonly used in New Zealand.

Groundwater discharge into lakes, also known as lacustrine groundwater discharge (LGD), is an oft-overlooked component of lake water budgets (Rosenberry et al. 2015). Methods for direct measurement of LGD include chemical and thermal tracer methods, and lakebed seepage meters. Application of these measurement techniques has shown that LGD can account for the majority of inflows for some lakes (e.g. Hamilton et al. (2006)). However, these methods are challenging to apply in many lakes due to difficulty of access to the lakebed combined with the slow rates but large areal extents over which LGD can occur. Thus, in many studies including in New Zealand, LGD is not measured directly but instead is modelled or derived from a water budget calculation (e.g. Thomas and Gibbs (2014)).

Groundwater discharge into wetlands is measured using the same techniques as for LGD (e.g. Lowry et al. (2007), Waddington et al. (1993), Rodellas et al. (2012)).

Groundwater discharge offshore, also known as submarine groundwater discharge (SGD), is increasingly recognised as an important component of the freshwater budget globally (Burnett et al. 2006) and in New Zealand (Coluccio et al. 2020). SGD is however one of the most challenging processes to measure directly because it is typically diffuse, can occur over large areas and multiple aquifers, and varies significantly through time (Coluccio et al. 2020). Techniques for directly measuring SGD include temperature sensing/profiling, measuring concentrations or fluxes of radon or other geochemical tracers, electromagnetic surveys, and seabed seepage meters (Burnett et al. 2006; Mulligan and Charette 2006). Despite a long-standing recognition of the need for more measurements of SGD in New Zealand (Science 2011), to date very few investigations have been undertaken (Stewart BT et al. 2018; Weymer et al. 2020).

2.4.1.4 Storage

The total volume of groundwater storage is typically estimated using geophysical survey approaches. Approaches used have included land-based microgravity measurements (Pool and Eychaner 1995), satellite-based gravimetry (Rodell et al. 2009; Wada et al. 2014), interferometric radar (Samsonov et al. 2010) and airborne electromagnetics (King et al. 2018). Note that all of these methods require inversion (modelling) of the geophysical signals to provide the estimates of groundwater volume, and hence are not direct measurement methods *sensu stricto*. The applicability of these methods for New Zealand groundwater systems has been reviewed by (Zemansky Gil 2015) and (Rawlinson Z 2013). With few exceptions (Samsonov et al. 2010; SkyTEM 2020) [Figure 9], these methods have not been employed in New Zealand due to costs, lack of availability of equipment, and/or challenges with measurement scale (Rawlinson Z 2013; Zemansky G and Devlin 2013).

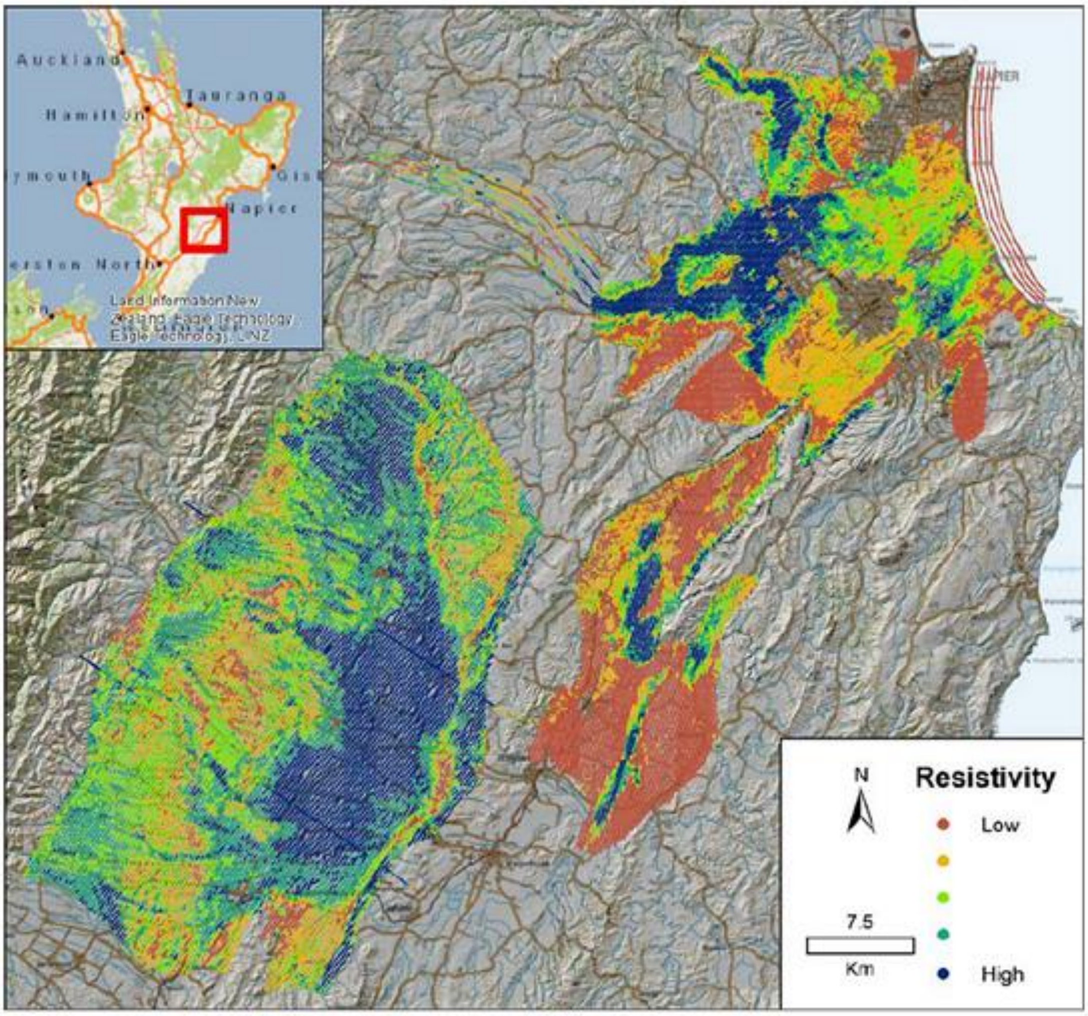

Figure 9: Preliminary resistivity estimates derived from airborne electromagnetic survey (SkyTEM) data over the Heretaunga Plains, Ruataniwha Plains and Otane and Poukawa Basins, Hawke's Bay region. Further modelling is required to interpret the occurrence of groundwater from the resistivity data. Source: (Moreau Moreau et al. 2020).

Changes in groundwater storage can be estimated using time-series surveys based on the above-mentioned geophysical techniques or, more simply, by measuring the depth to groundwater level in combination with assumptions of aquifer extent and porosity (Moreau M 2020). The approach is to identify a number of indicator wells, for which groundwater level variations are considered indicative of the changes occurring over the whole aquifer or IOU, and then apply the following equation:

Equation 1

Change in groundwater volume (m^3) = Change in indicator well water level (m) x Aquifer areal extent (m^2) x Aquifer Porosity (unitless)

To aid calculations using the equation above, aquifer extents have been recently updated (Figure 7) and classified in terms of main hydrogeological properties (White P et al. 2019), and estimates of aquifer porosity (Westerhoff et al. 2017) and depth to hydrogeological basement (Westerhoff, Tshcritter, et al. 2019) have also recently been tabulated at the national scale (Figure 10). New Zealand standard procedures for measuring the depth to groundwater are provided in Daughney C et al. 2006 and National Environmental Monitoring Standards 2019.

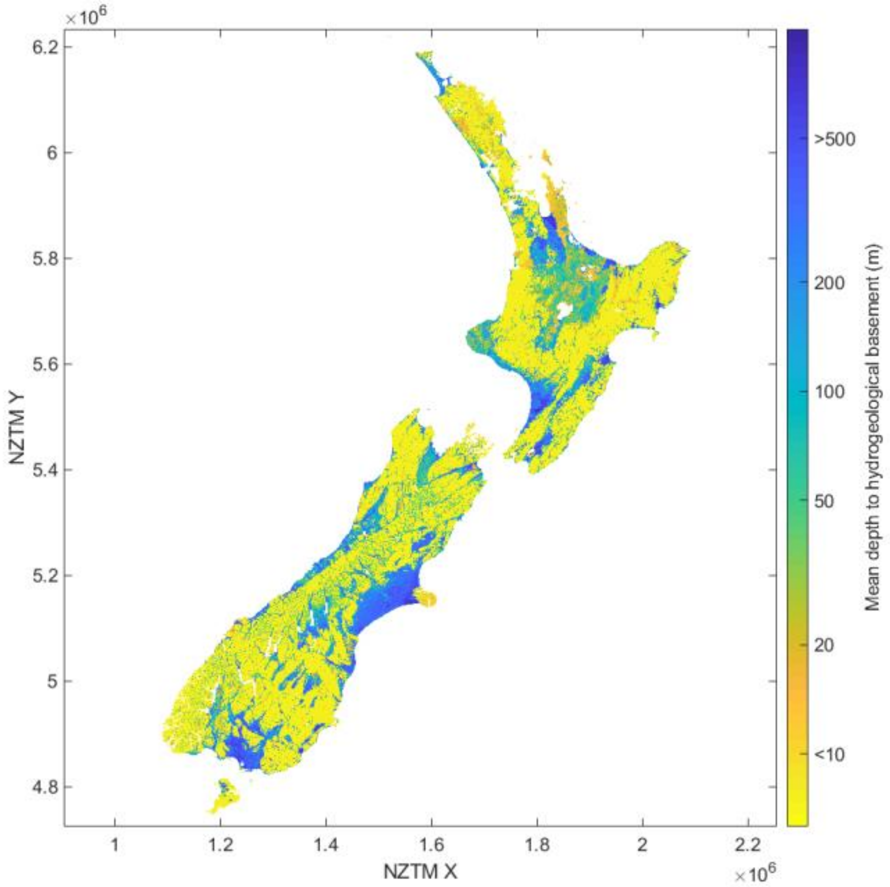

Figure 10: Mean modelled depth to hydrogeological basement, defined as the depth at which the primary porosity and permeability of the geological material is low enough that fluid volumes and flow rates can be considered negligible. Source: Westerhoff, Tshcritter, et al. (2019).

2.4.2 Modelling

Many groundwater models have been developed for New Zealand, albeit few for the scale of the whole country. It is beyond the scope of this report to review and compare each of the available models but, in summary, they collectively represent a range of tools and approaches that can be used to estimate current, past and future groundwater levels, flows and exchange fluxes with soil moisture, surface water bodies and the sea.

Along with discussing groundwater flow models, we discuss four common approaches that are used to model groundwater concentrations, all of which aim to estimate the concentrations of substances that have not been directly measured at the required locations and/or times. One approach is to use interpolation to estimate contaminant concentrations in between wells or other sampling points at which measurements have been made (Figure 11). The second approach is to apply machine-learning methods to identify patterns in the variations amongst the concentrations of several different elements or compounds across various sites, thereby enabling site-specific estimation of the concentrations of substances that have not been measured from the concentrations of those that have (Daughney C et al. 2015; Iwashita et al. 2018). The third approach is to combine process-based or machine-learning methods with interpolation to improve the accuracy of estimation of contaminant concentrations in between measuring points (Rissmann CWF et al. 2019; Wilson et al. 2020). For example, predictors such as soil type, geology, land use and climate have been applied alongside well-specific groundwater quality measurements to improve national scale maps of aquifer redox conditions (Figure 12). The fourth approach is to undertake mass transport modelling as discussed under the Internal Flows subsection below. This fourth modelling approach takes specific account of groundwater flow directions along with reaction rates when simulating contaminant concentrations within the model domain, whereas the first three modelling approaches listed in this paragraph do not.

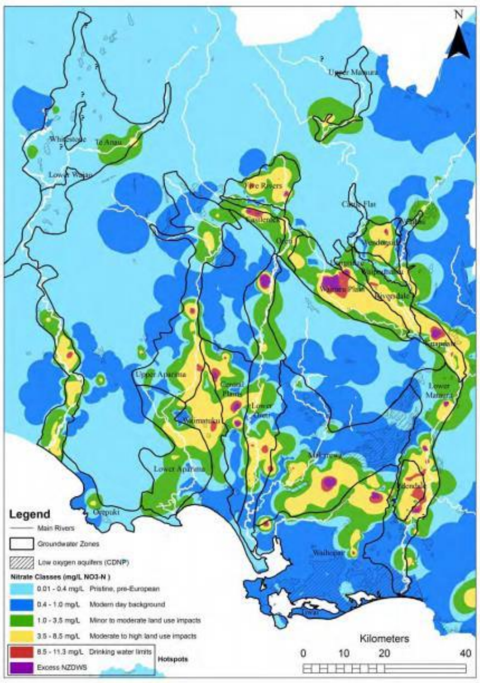

Figure 11: Interpolated nitrate-nitrogen concentration in the Southland region based on measurements made at 710 monitoring sites between 2007 and 2012. Source: Rissmann C (2012).

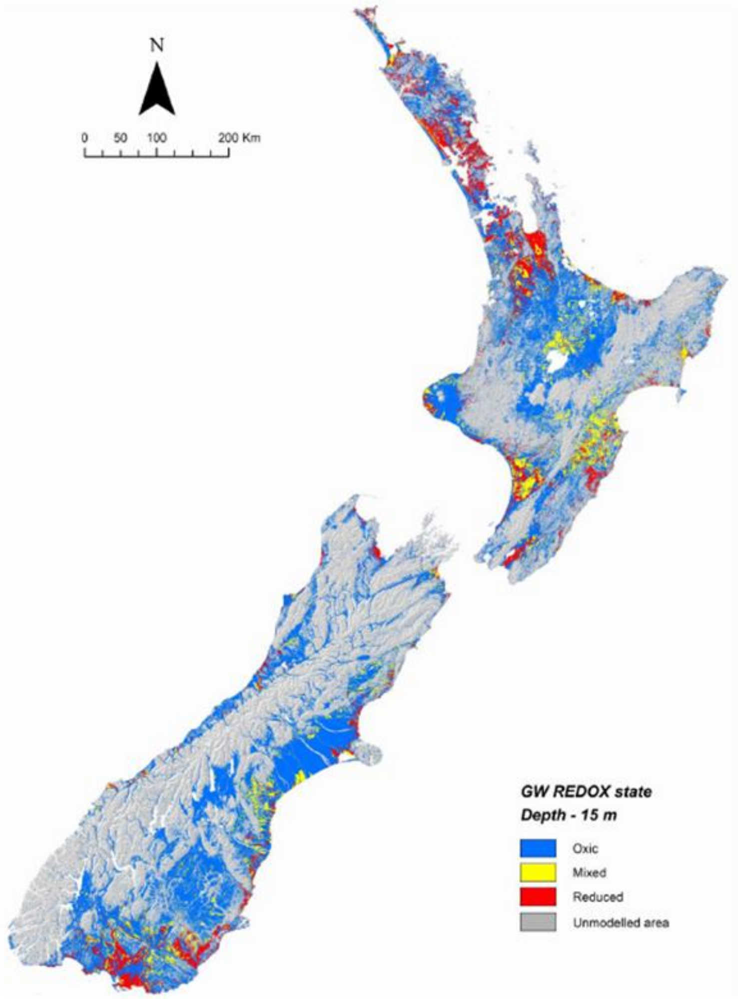

Figure 12: Modelled groundwater redox condition at 15 m depth based on a statistical learning approach applied to a range of predictor datasets such as soil type, geology and elevation. Source: Wilson et al. (2020).

2.4.2.1 Inflows

Groundwater recharge from soil drainage (i.e. LSR) has been modelled at the national scale (Figure 13). The TopNet model provides estimation of soil moisture drainage (i.e. LSR) at an hourly time step and can be run for various spatial resolutions (e.g. approximately 60,000 catchments at Strahler 3) (Bandaragoda et al. 2004). The National Groundwater Recharge Model (NGRM) estimates LSR at a 1 km grid size with a monthly time step (Westerhoff, White, Rawlinson 2018). The IrriCalc model (Bright et al., 2018) estimates LSR for potentially irrigable areas using a daily time step at relevant VCSN points (a grid of 0.05 lat/long arc degrees) (Westerhoff, Dark, et al. 2019). These national-scale estimates of LSR can be applied for water accounting purposes if more localised measurements or models are not available (Johnson P et al. 2019; Westerhoff, Dark, et al. 2019).

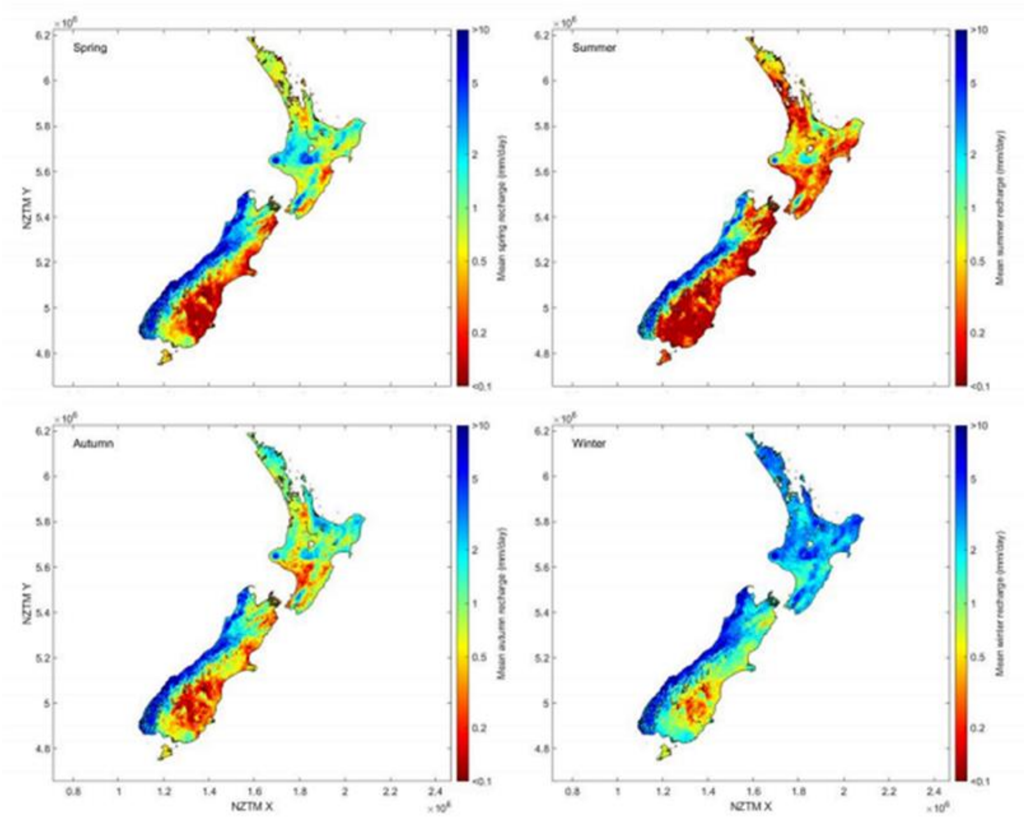

Figure 13: Mean modelled seasonal rainfall recharge to groundwater (i.e. LSR), based on the average of values from the TopNet, NGRM and IrriCalc models. Spring: Sept-Nov, Summer: Dec-Feb, Autumn: Mar-May, Winter: June-Aug. Source: Westerhoff, Dark, et al. (2019).

Groundwater recharge from river seepage (i.e. SWR) has not been quantified in terms of volume or rate at the national scale, but preliminary national-scale maps of the locations of such occurrences have been generated (Westerhoff, Dark, et al. 2019). One mapping approach is based on the Random Forest technique (Yang et al. 2019) (Figure 14). A second mapping approach is based on a National Water Table (NWT) model (250 m grid, hourly time step), which provides relative but not absolute magnitudes of exchange fluxes in addition to identifying the locations where they occur (Westerhoff, White, Miguez-Macho 2018).

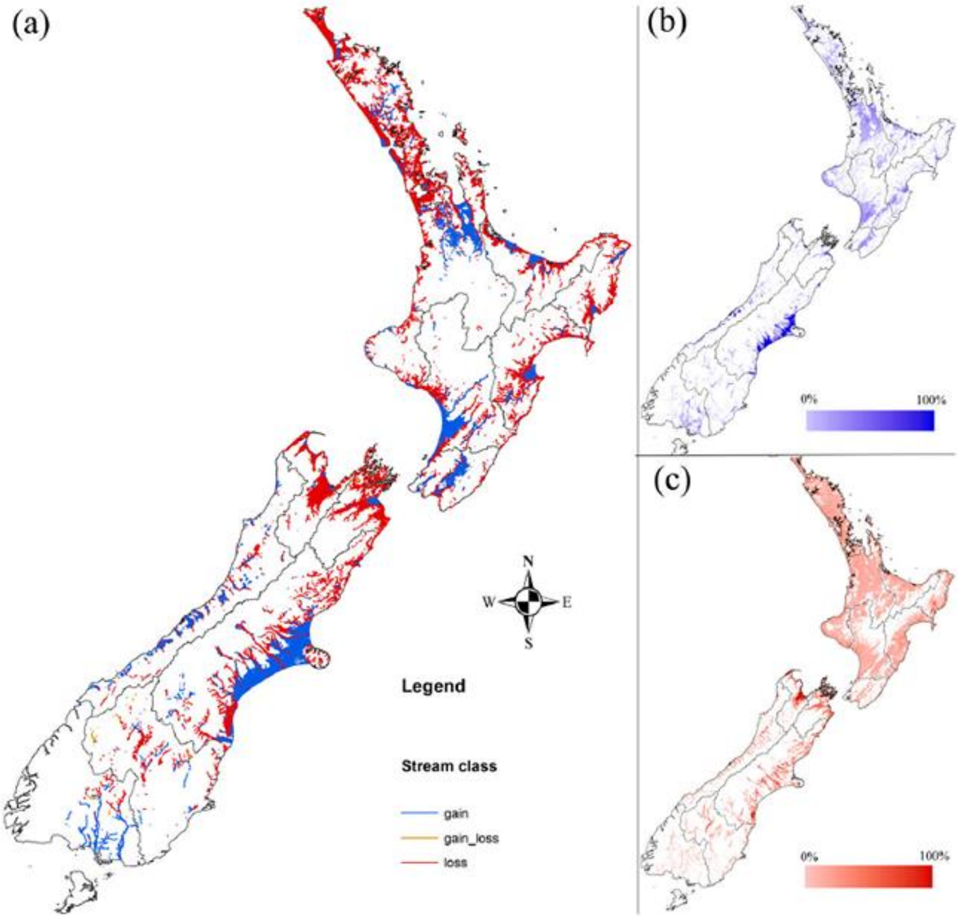

Figure 14: National classification of gaining and losing stream reaches. a) predicted gain and loss reaches where 'loss' means the river water is recharging groundwater, 'gain' means groundwater is discharging into the river, and 'gain_loss' means the reach gain either recharge to groundwater or receive discharge from groundwater variably over time (reaches are not mapped they could not be assigned to one of these three categories). b) probability distribution of 'loss' reaches. c) probability distribution of 'gain' reaches. Source: Westerhoff, Dark, et al. (2019).

In addition to the above-listed national-scale groundwater recharge models, there are many groundwater recharge models that have been developed for more localised scales. Some of these local-scale models are intended specifically for estimation of LSR (e.g. White P et al. (2003), Bekesi and McConchie (1999), Baalousha Husam (2009)), whereas other applications involve the incorporation of models of LSR and/or SWR within more comprehensive models of the groundwater system (see *Flows* below).

Of note, all of the above-mentioned national- and local-scale recharge models are based on precipitation and evapotranspiration, often derived from the VCSN, which means that coupling to weather and/or climate models enables generation of LSR and SWR forecasts if so required for water accounting.

There are a variety of contaminants that can be carried into the groundwater along with water inflows. The inflow pathways include soil drainage and/or irrigation return flow (together referred to as land surface recharge, LSR), and surface water recharge (SWR) from rivers, lakes, wetlands or other surface water bodies (Johnson PJ 2019). Contaminants can also be introduced directly into the groundwater system, e.g. via flows from septic tanks, soak holes, tile fields or injection wells (Freeze and Cherry 1979; Johnson PJ 2019). Contaminants of concern introduced to New Zealand groundwater systems via the above-listed pathways include nutrients (Morgenstern and Daughney 2012; Collins S et al. 2017), pathogens (Close M et al. 2008; Weaver et al. 2016), heavy metals (Speir et al. 2003), pesticides (Morgenstern and Daughney 2012; Close ME et al. 2021) and a wide range of emerging organic contaminants (Moreau Magali et al. 2019; Close ME et al. 2021). Seawater can also be drawn into aquifers due to sea level rise and/or over-abstraction of groundwater, which can result in contamination of fresh groundwater by salts of marine origin (Werner et al. 2013).

Contaminant inflows can be estimated from the flux of water entering the groundwater system and the concentration of the contaminant within the inflowing water (Equation 2). An overview of approaches for measuring contaminant concentration is provided above. Approaches for measuring water inflows (recharge) to groundwater are covered in Section 2.3.1 and include lysimeters for quantifying LSR (e.g. Duncan et al. (2016), White PA et al. (2013)) and concurrent gaugings for quantifying SWR (Cameron S and White 2004; Baalousha HM 2012a). Note that this approach only provides an estimate of contaminant inflow to the groundwater system at the specific location and time that the concentration and water flow measurements were made; extension of such measurements to whole-of-aquifer scale requires some form of modelling and hence is discussed in under the Modelling subsection.

Equation 2

Contaminant inflow (g/day) = Contaminant concentration (g/m^3) x Water inflow (m^3/day)

The fluxes of contaminants that leach through the soil zone are usually assumed to be equivalent to the inflows to the groundwater system. This means that the approaches described in Section 2.3.2 for modelling contaminant outflows from soil are also used to model contaminant inflows into groundwater. As noted above, such contaminant leaching models are already available for nutrients and bacteria for New Zealand soils. Where models of contaminant leaching from the soil zone are not available, groundwater investigations often apply assumed loading values or leaching rates adopted from field studies, usually expressed as kilograms per hectare per year for particular land uses (e.g. (White P et al. 2007; Toews M and Gusyev 2012). Leaching rates of nutrients through New Zealand soils have been assessed in many investigations, including at the national scale (Parfitt et al. 2006; Parfitt et al. 2008; Parshotam et al. 2012), and N leaching from livestock has been mapped nationally (Figure 15). Some information on leaching of bacteria and viruses into New Zealand groundwater systems is also available (e.g. Weaver et al. (2016), Pang, McLeod, Aislabie, Šimůnek, et al. (2008), Moore et al. (2010)). However, there are fewer comprehensive studies for the leaching rates of other types contaminants through New Zealand soils. In those cases where leaching rates for contaminant inflows to groundwater have not been previously modelled or measured in the field, it is an option to treat the contaminant inflows as a spatio-temporally variable parameter to be optimised during groundwater model calibration, by matching measured and modelled concentrations in the groundwater system (Toews M and Gusyev 2012; Weir et al. 2013).

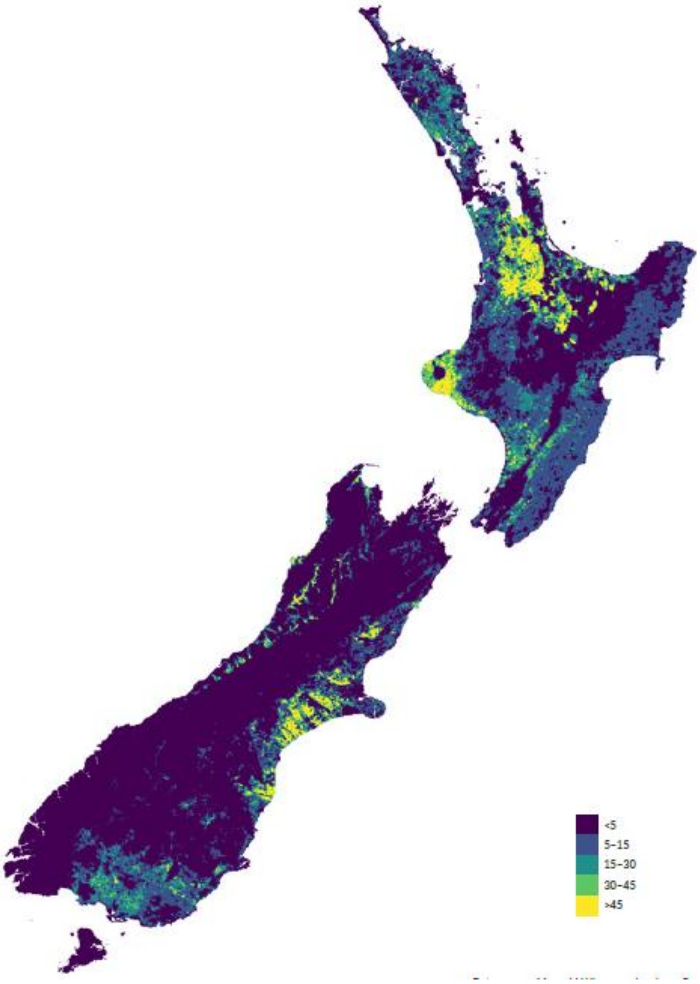

Figure 15: Modelled nitrate-nitrogen leaching from livestock, 2017 (kg N per ha per year). Source: StatsNZ (2019)..

2.4.2.2 Internal flows

It is commonplace to develop numerical models that represent most key groundwater processes, not only simulating flows, but also recharge and discharge as key boundary conditions, along with storage volumes and changes in the calculated groundwater balance. Routinely used groundwater modelling tools include MODFLOW, FEFLOW, SWAT and others. Key considerations in groundwater modelling include selection of software, model grid configuration and discretization, and whether the model is steady-state or time-stepping (transient). Increasingly, models of groundwater systems are integrated with or loosely coupled to models of the surface water and climate systems, so that the hydrological system can be simulated holistically across all of its interacting parts (e.g. Durney et al. (2016), Blyth et al. (2018), Rakowski (2018)), despite the recognised modelling challenges involved (Elliott et al. 2017). Furthermore, groundwater flows are commonly modelled simultaneously with the fate and transport of contaminants in the groundwater system.

The NWT model (Westerhoff, White, Miguez-Macho 2018), described above, is presently the only national-scale groundwater model that has been developed for New Zealand. Originally developed to model the depth to the groundwater table, the NWT model has since been applied to map the locations and relative magnitudes of groundwater-surface water exchange (see above), but it has not been applied to determine groundwater flow velocities, discharge to the sea, interaction with lakes, or other aspects of groundwater system dynamics.

Aside from the national-scale NWT model, many groundwater flow models have been developed for specific parts of New Zealand. The scales of these existing groundwater models range from multi-catchment to catchment to sub-catchment or an even smaller area of interest. A recent review indicates that groundwater models of some type have been developed for most regions (Figure 16), though groundwater flows have not been simulated in all cases (Johnson P et al. 2019). Examples of areas with existing numerical groundwater models capable of simulating flows, recharge, discharge and storage include the area between the Rakaia and Waimakariri Rivers in Canterbury (Weir 2018), the Lake Rotorua catchment in the Bay of Plenty (Daughney CJ et al. 2015), the Ruamahanga catchment in the Wellington region (Blyth et al. 2018), the Ruataniwha, Poukawa and Heretaunga basins in Hawke's Bay (Baalousha H et al. 2010; Cameron S et al. 2011; Baalousha HM 2012b; Rakowski 2018)), the Wairau catchment in Marlborough (Wöhling et al. 2018), the Waimea Plains and Motueka catchments in the Tasman region (Hong and Thomas 2006; Hong et al. 2010), and the Aparima catchment in Southland (Johnson PJ 2019). Given their greater resolution and representation of soil, aquifer and groundwater features, where available such localised models should be considered instead of national-scale models for use in water accounting.

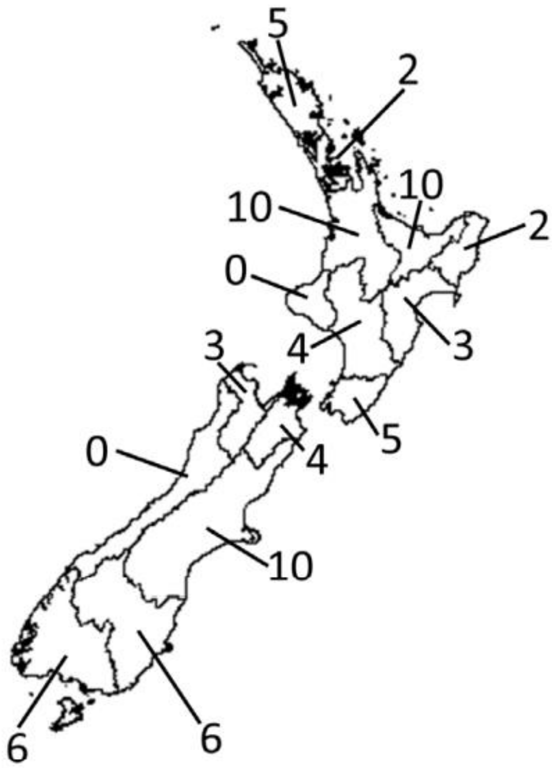

Figure 16: Number of groundwater basins within each region for which some type of groundwater model is presently available, though not all of these existing models are capable of simulating groundwater flow. Source: Johnson PJ (2019)

Internal flows of groundwater can also be assessed with the assistance of age tracers. Age tracers are substances such as tritium, chlorofluorocarbons, sulphur hexafluoride and carbon-14 that have known historical variations in their input to the hydrological system via rainfall, and which can therefore be used to infer the residence time and/or transport velocity of a groundwater sample (Stewart M and Morgenstern 2001; Daughney CJ et al. 2010). The age tracer approach firstly requires measurement of their concentrations, which is performed by collection of a groundwater sample according to standard procedures (Daughney C et al. 2006; National Environmental Monitoring Standards 2019) followed by laboratory analysis (see Daughney CJ et al. (2010)). Secondly, some type of model is applied to infer the age distribution from the measured concentration of the tracers. Various types of lumped parameter models have been widely used in New Zealand for this purpose (Stewart M and Morgenstern 2001), including for sites in the National Groundwater Monitoring Programme (Daughney CJ et al. 2010; Morgenstern and Daughney 2012) as well as several regional or catchment studies (e.g. Morgenstern et al. 2018, Daughney C et al. 2015, Morgenstern, Daughney, et al. 2014). A growing number of studies have evaluated the age distribution by fitting numerical groundwater models to the observed age tracer data (Toews M and Gusyev 2012; Gusyev et al. 2013; Weir et al. 2013; Daughney CJ et al. 2015; Toews MW et al. 2016; Knowling et al. 2020). Whether interpretation is based on an LPM or a numerical groundwater model, the modelled age distribution is typically reported in the form of its mean and some measure of its distribution, which together provide information about internal flows of groundwater that have converged at the sampling point.

Contaminant flows within the groundwater system, i.e. along groundwater flow paths, can be assessed in-situ at a localised scale using tracer tests. These tests involve injection of a known mass of the contaminant of interest into the groundwater system, along with a conservative tracer, and measurement of their appearance over time at down-gradient wells or sampling points, usually under natural (i.e. non-pumped) groundwater flow conditions. Several such tests have performed in New Zealand, providing information about groundwater transport rates of contaminants such as nitrate (Burberry et al. 2013; Dann et al. 2013), phosphorus (Gray et al. 2015), heavy metals (Pang and Close 1999), pesticides (Pang and Close 2001), viruses (Sinton et al. 2000; Sinton et al. 2005; Weaver et al. 2013) and bacteria (Sinton et al. 2000; Sinton et al. 2005; Weaver et al. 2013). Collectively these studies show that the local contaminant transport rate depends on many factors such as the characteristics of the contaminant (e.g. dissolved vs. colloidal, reactive vs. non-reactive), the hydraulic properties of the porous medium (e.g. effective porosity), the chemistry of the groundwater (e.g. pH, salinity, organic carbon content), and whether contaminants are present singly or in combination. Ex-situ tracer tests can also be performed, whereby the contaminants of interest are passed through an intact column of porous medium that has been extracted from the aquifer (Wall et al. 2008; Walshe et al. 2010) but such tests are often performed at flow velocities and/or under chemical conditions different from natural conditions and hence results may not translate directly to native groundwater (Vereecken et al. 2011).

Contaminant flows within the groundwater system can also be assessed with the aid of age tracers. However, interpretation of residence time or groundwater flow rates from age tracer data requires some form of modelling and hence this approach is discussed in the Modelling subsection below.

Mass transport modelling is routinely applied to simulate the inflows, internal flows, outflows and spatiotemporal distributions of contaminants in groundwater systems (Bethke 2007). Transport of single contaminant undergoing a limited number of reactions can be simulated with software packages such as MODFLOW-MT3D or FEFLOW, whereas simulation of the transport of several contaminants and more complex reactions involves coupling a geochemical reaction model with a simulation of advective-dispersive groundwater flow with the aid of one of several computer programs developed for this purpose (Parkhurst and Appelo 1999; Xu et al. 2004; Parkhurst et al. 2010; Bethke et al. 2021).

As noted in Section 2.4.2.1, many groundwater models have been developed for New Zealand catchments (Johnson P et al. 2019). Models that simulate the transport of a contaminant (usually nitrate) within the groundwater system have been developed for several parts of the country including selected catchments in Southland (Thomas 2012), Waikato (Toews M and Gusyev 2012; Weir et al. 2013), the Bay of Plenty (White P et al. 2007; White P et al. 2016), Wellington (Rawlinson ZJ et al. 2017; Blyth et al. 2018) and Hawke's Bay (White P and Daughney 2004; Baalousha H 2013). Routinely used groundwater modelling tools include MODFLOW, FEFLOW and SWAT. Most of these models simulate a range of contaminant transport processes including contaminant inflows, internal flows, discharge and reaction, along with varying degrees of integration with surface water bodies (Johnson P et al. 2019). Other models have also been developed to simulate contaminant transport within the wider hydrologic system, albeit often with a somewhat simpler representation groundwater processes (Rutherford et al. 2009; Oehler and Elliott 2011; Parshotam et al. 2012; Semadeni-Davies et al. 2015). It is beyond the scope of this report to review and compare these available contaminant transport models.

Modelled residence times and/or water age distributions can also be used to assess the internal flows of contaminants within a groundwater system. For example, the concentrations of contaminants can be compared between samples of different groundwater age, providing insight into the flows of groundwater that carry them (Morgenstern, Daughney, et al. 2014).

2.4.2.3 Outflows

Groundwater discharge to rivers, lakes, wetlands and the sea is not generally modelled in isolation of other processes but rather is simulated using holistic groundwater flow models as described in the previous section.

At the national scale, locations of groundwater discharge into rivers have been mapped using TopNet and the NWT model (see Figure 13) but the rates and fluxes have not been quantified in absolute terms (Westerhoff, Dark, et al. 2019). These models can also simulate national and regional groundwater outflows to the sea at hourly and daily time-steps (Griffiths et al. 2021).

Most of the existing local-scale models described in the previous section provide estimates of groundwater discharge to surface water and/or the sea where relevant to the area being modelled. For example, locations and fluxes of groundwater discharge to the sea have been assessed in the Heretaunga Plains (Rakowski 2018), groundwater discharge into Lake Rotorua has been evaluated under baseflow conditions (Daughney CJ et al. 2015), and groundwater discharge into rivers has been simulated in several models (Hong and Thomas 2006; Hong et al. 2010; Cameron S et al. 2011; Daughney CJ et al. 2015; Rakowski 2018).

Contaminant outflows from the groundwater system can occur via discharge into lakes, rivers, wetlands and the sea. The measurement approach requires assessment of contaminant concentration and water outflows (Equation 3). Methods for measuring outflows of water from the groundwater system are listed in Section 2.4.1 and include concurrent gaugings (Cameron S and White 2004; Baalousha HM 2012a), radon mass balance (Martindale Heather et al. 2016; Morgenstern et al. 2018), temperature profiling (Donath et al. 2015; Moridnejad et al. 2020) and seepage meters (Burnett et al. 2006; Coluccio et al. 2020) As for measurements of contaminant inflows, the results of such assessments of contaminant outflows apply only to the specific locations and times that the contaminant concentrations and water fluxes are measured.

Equation 3

$$\text{Contaminant outflow (g/day)} = \text{Contaminant concentration (g/m}^3\text{) x Water outflow (m}^3\text{/day)}$$

2.4.2.4 Storage

At the national scale, changes in groundwater storage can be modelled with TopNet (Griffiths et al. 2021) or indirectly simulated based on the groundwater level from the NWT model (Westerhoff, White, Miguez-Macho 2018) coupled with estimates of aquifer volume and porosity as per Equation 1. The TopNet and NWT produce spatially resolved outputs at the hourly and daily time-steps, respectively, and can be coupled to weather and climate models to generate forecasts and projections of change in water storage across different time horizons for water accounting purposes.

At a local scale, the existing groundwater models described in previous sections and summarised in (Johnson P et al. 2019) produce itemised groundwater budgets as a routine type of output because this allows assessment of the model’s convergence. An example of a calculated groundwater budget is shown in Table 2, developed for the Heretaunga Plains (Rakowski 2018). Of note is that some line items in the water balance are based on measurements, other line items are based on models, and the discharge to the sea has neither measurements nor models and so is estimated by balancing the total inflows and total outflows, meaning that the average annual change in storage is assumed to be zero for the time period of interest.

Table 2: Average annual water budget for the Heretaunga Plains groundwater system, based on the period 2005-2015. Source: (Rakowski 2018).

	Type	Description	Mm³/year	L/s	
INFLOWS	River Recharge (to groundwater)	Total river recharge to groundwater (based on observed major river losses by HBRC)	**188.6**	**5,980**	71%
		including:		4,400	
		Ngaruroro loss	138.8	780	
		Tukituki losing	24.6	800	
		Tutaekuri losing	25.2		
	Land Surface Recharge from rainfall	LSR calculated by Aqualinc for the unconfined area	78.5	2,489	29%
	TOTAL INFLOWS		**267.1**	**8,469**	
OUTFLOWS	Spring discharges	Measured summer discharges	111.0	3,520	42%
	Groundwater pumping	Some data and estimated from demand modelling	78.1	2,475	29%
	Sea discharge	No observations	78.0	2,474	29%
	TOTAL OUTFLOW		**267.1**	**8,469**	

Groundwater storage can also be estimated using the concentration of tritium measured in a stream water sample (other age tracers are gaseous and hence cannot be straightforwardly applied to surface water samples due to complications introduced by air-water exchange) (Stewart M and Morgenstern 2001). The approach is to analyse the tritium concentration in a sample of stream water collected under baseflow conditions, which is assumed to be dominantly composed of groundwater. Thus, the inferred age distribution of the sample, combined with the stream flow rate, can be used to infer the total volume of the groundwater store that is feeding the baseflow (Morgenstern, Begg, et al. 2014; Daughney C et al. 2015).

As for other components of the hydrological system, evaluation of contaminant stocks and flows in groundwater involves determination of: contaminant inflows from other parts of the hydrological system or direct to groundwater; the pathways and rates of contaminant transport by flowing groundwater; extent of any transformations or reactions that add or remove the contaminant within the groundwater system; and contaminant discharges to other parts of the hydrologic system. Contaminant inflows and outflows are typically assessed by combining information about contaminant concentration together with other data about water fluxes.

Concentrations of substances of interest are normally measured by extracting a sample of groundwater from the subsurface, which is then analysed ex situ, usually at a chemical laboratory. Standard protocols are in use for sampling the saturated zone as part of routine groundwater quality monitoring in New Zealand (Daughney C et al. 2006; National Environmental Monitoring Standards 2019). Monitoring of groundwater quality in the vadose zone is less routine in New Zealand, but sampling protocols have also been developed (Fares et al. 2009; Singh G et al. 2018). Standard laboratory and/or field analytical protocols are available the most commonly monitored groundwater quality indicators and are applied for samples from the saturated and vadose zones. Data from routine regional and national groundwater quality networks are available online (GNS Science nd; Land Air Water Aotearoa nd), comprising approximately 1,000 long-term monitoring sites across New Zealand (Figure 17). Note that the analysis of a sample only provides information about the chemical composition of groundwater immediately around the well or sampling point, and only at the time the sample was collected.

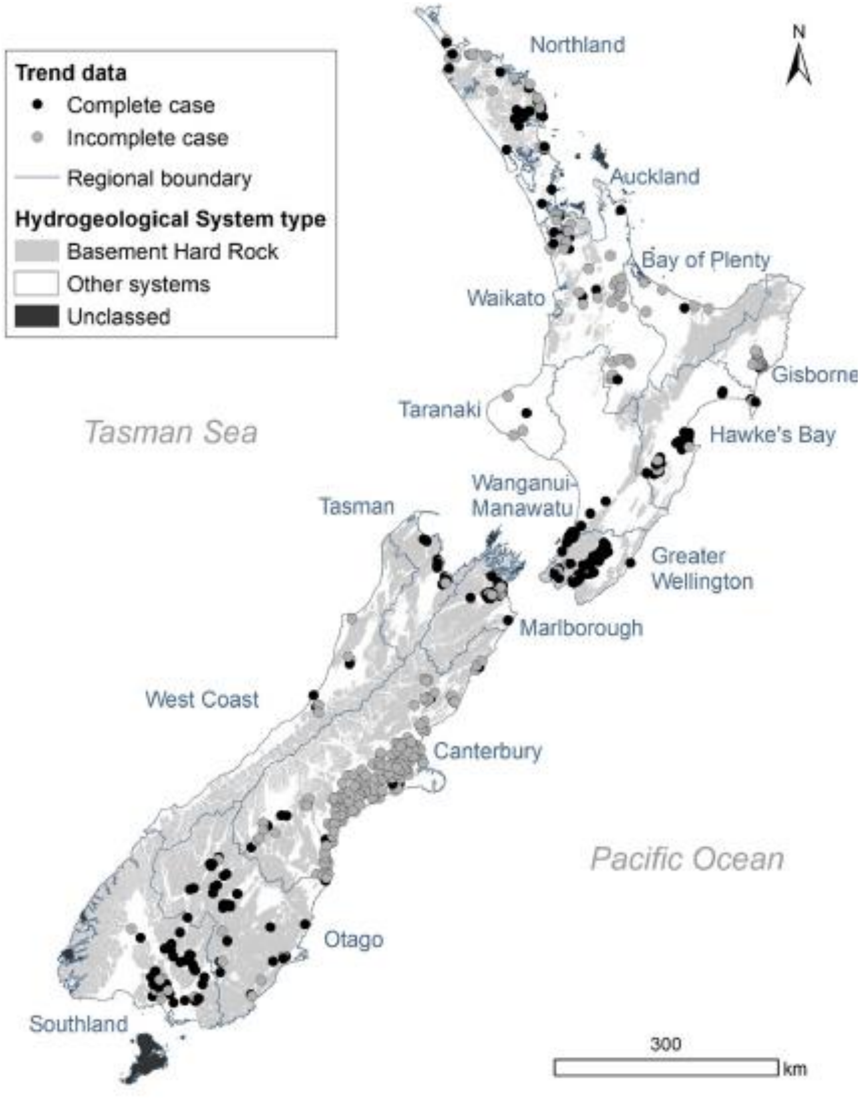

Figure 17: Groundwater monitoring sites having complete (black dots) or incomplete (grey dots) time-series for quarterly measurements of commonly analysed parameters over the period 2005 to 2014. Source: (Moreau M and Daughney 2020).

As opposed to collection of samples, some geophysical approaches can also be applied to assessing some aspects of groundwater quality in situ, particularly salinity (Duncan et al. 2016; King et al. 2018; Moreau Moreau et al. 2020). Unlike the collection of groundwater samples from specific sampling points, these geophysical methods can provide more spatially continuous information about groundwater chemistry across an aquifer. Note however that these approaches require interpretation of groundwater quality based on the geophysical signal and hence are not direct measurements.

Two main modelling approaches are available for estimation of the total stocks of a contaminant in a groundwater system, given stocks cannot be measured directly. The first approach is to derive an average concentration of the contaminant across the whole aquifer, based on interpolation of the measurements at individual wells, then multiply by the total volume of groundwater derived from one of the methods described in Section 2.4.1.4. The second approach is to obtain the total mass of contaminant from a numerical transport model, which would typically produce this information as part of checking the mass balance during convergence testing.

Storage or stocks of contaminants in a groundwater system cannot be measured directly and so are estimated through modelling (see below).

2.4.2.5 Reactions

A variety of physical, chemical and biological processes can affect the mass of certain contaminants in the groundwater system. Some reactions add contaminants to groundwater whereas other reactions remove contaminants from groundwater. Determination of the rates of these reactions and the extent to which they have or will affect stocks and flows are therefore important aspects of contaminant accounting.

The natural process of water-rock interaction can add certain contaminants to the groundwater system. This occurs when constituents of the porous medium are solubilised into the groundwater via mineral dissolution or desorption from mineral surfaces (Langmuir 1997). The rates of many such reactions are controlled by physicochemical conditions in the aquifer, such as temperature, salinity, pH, redox condition, etc (Langmuir 1997). Some of these reactions occur purely abiotically, for example under geothermal conditions, which can introduce contaminants such as mercury, arsenic and selenium into groundwater (Smedley and Kinniburgh 2002; Holley et al. 2010; Floor and Roman-Ross 2012). Other reactions are catalysed by naturally resident aquifer microorganisms that gain energy from these reactions (Langmuir 1997; Chapelle 2000). An example is the release of arsenic into groundwater concomitant with the microbially mediated dissolution of iron oxide minerals that can occur under oxygen-free (reducing) conditions (Chapelle 2000; Smedley and Kinniburgh 2002; Islam et al. 2004). The rates of weathering reactions that enable phosphorus to accumulate in soil drainage have been generalised for different soil types at a national scale (Parfitt et al. 2006). Phosphate is also often associated with iron oxide minerals and, like arsenic, can be released into groundwater due to microbially mediated reductive dissolution (Langmuir 1997; Chapelle 2000), and hence phosphate concentrations often increase with declining oxygen concentrations, as is commonly observed with increasing groundwater age and distance along a flow path (Daughney CJ et al. 2010; Morgenstern and Daughney 2012). Other potential contaminants that can be released via microbially mediated processes include manganese, mercury, chromium, and several others (Langmuir 1997; Chapelle 2000). Note that these processes occur naturally, but under certain conditions the compounds released into groundwater can accumulate to potentially harmful levels, hence their classification as contaminants in this report.

Natural reactions within an aquifer can remove contaminants from groundwater too. Notable among these is denitrification, the process by which nitrate-nitrogen is converted into more reduced forms of N such as nitrite, nitrous oxide and nitrogen gas (Chapelle 2000). Denitrification is favoured under reducing conditions (Langmuir 1997; Chapelle 2000) and hence nitrate concentrations are often observed to decrease in the absence of oxygen, as often observed with increasing groundwater age and distance along a flow path (Daughney CJ et al. 2010; Morgenstern and Daughney 2012). Some organic contaminants can be broken down by aquifer microbes (Chapelle 2000; Pang and Close 2001). Contaminants such as arsenic, phosphate, selenium and heavy metals can be removed from groundwater through co-precipitation with iron or manganese oxyhydroxide minerals, for example if a groundwater flow path crosses from oxygen-poor to oxygen-rich conditions (Langmuir 1997; Chapelle 2000). Viruses and bacteria are removed from groundwater due to die-off (Sinton et al. 2000; Wall et al. 2008). Particulate contaminants including viruses and bacteria can also be affected by filtration, i.e.

the restriction of movement through pore spaces that are too small for their passage, but note that this does not always impede their rate of transport and indeed can cause them to move at faster than the average advective velocity of the groundwater due to pore size exclusion (Pang and Close 1999).

Conducting a tracer test is the typical approach for measuring the rates of such reactions in the groundwater system. The contaminant of interest is injected into the groundwater system along with a conservative tracer such as chloride or bromide; differences in the mass of recovered contaminant compared to the conservative tracer can be used to infer reaction rates (Sinton et al. 2000; Pang and Close 2001; Wall et al. 2008; Burberry et al. 2013; Dann et al. 2013). While tracer tests are commonly performed between wells, so-called push-pull tests can be performed by injecting the contaminant and conservative tracer into a single well and then extracting a sample from the same well by pumping at a later time (Istok et al. 1997). An alternative to performing inter-well or single-well tracer tests in the field is to extract aquifer materials and conduct column tests or batch reaction tests in the laboratory, although these methods may not precisely reproduce the biogeochemical and hydrological conditions of the aquifer and hence may yield biased estimates of reaction rates.

There are two additional techniques that are available for evaluating denitrification in particular. First, the excess N gas (N_2) approach involves measurement of dissolved argon, neon and N_2 in a groundwater sample, which enables the amount of dissolved N_2 produced as an end-product of the denitrification reaction to be measured distinctly from the amount of dissolved N_2 that originated from the atmosphere (Martindale H et al. 2019). Second, measurement of stable isotope signatures of nitrate can be used to detect shifts caused by denitrification (Clague et al. 2015). Both of these techniques provide information on the total mass of nitrate that has been transformed, but additional information on groundwater flow velocity or age is required to infer the rate of reaction (Martindale H et al. 2019).

Rates of reaction can also be assessed with the aid of age tracers but this requires some form of modelling and hence this approach is discussed in the Modelling subsection below.

The fluxes of contaminants that leach through the soil zone are usually assumed to be equivalent to the inflows to the groundwater system. This means that the approaches described in Section 2.3.2 for modelling contaminant outflows from soil are also used to model contaminant inflows into groundwater. As noted above, such contaminant leaching models are already available for nutrients and bacteria for New Zealand soils. Where models of contaminant leaching from the soil zone are not available, groundwater investigations often apply assumed loading values or leaching rates adopted from field studies, usually expressed as kilograms per hectare per year for particular land uses (Toews M and Gusyev 2012; White P et al. 2016). Leaching rates of nutrients through New Zealand soils have been assessed in many investigations, including at the national scale (Parfitt et al. 2006; Parfitt et al. 2008; Parshotam et al. 2012), and N leaching from livestock has been mapped nationally (Figure 15). Some information on leaching of bacteria and viruses into New Zealand groundwater systems is also available (Pang, McLeod, Aislabie, Simunek, et al. 2008; Moore et al. 2010; Weaver et al. 2016). However, there are fewer comprehensive studies for the leaching rates of other types contaminants through New Zealand soils. In those cases where leaching rates for contaminant inflows to groundwater have not been previously modelled or measured in the field, it is an option to treat the contaminant inflows as a spatio-temporally variable parameter to be optimised during groundwater model calibration, by matching measured and modelled concentrations in the groundwater system (Toews M and Gusyev 2012; Weir et al. 2013).

Modelled outflows from the groundwater system into surface water bodies are treated as inflows to those bodies. Otherwise, modelled outflows from the groundwater system represent discharge to the sea.

Outflows of contaminants from the groundwater system are usually estimated using a numerical transport model of the type described in the Internal flows section above. This approach has been applied to estimate N inflows to streams and lakes in parts of the Waikato (Toews M and Gusyev 2012; Weir et al. 2013), Bay of Plenty (Rutherford et al. 2009; White P et al. 2016), Hawke's Bay (White P and Daughney 2004; Baalousha H 2013) and Wellington Regions (Rawlinson ZJ et al. 2017).

Modelled residence times and/or water age distributions can also be used to assess the outflows of contaminants from a groundwater system. Measurement of an age tracer together with the concentrations of contaminants in the groundwater outflow, such as in a stream sample collected under baseflow conditions, can indicate the residence time of the contaminant in the groundwater system (e.g. Morgenstern et al. (2010)). Of particular importance for accounting purposes, the modelled age distributions can also be used for forecasting the contaminant outflows in the future (i.e. 'load to come' (Schiel and Howard-Williams 2016)) by coupling age-tracer-derived residence times with information on the concentrations of contaminants in samples of different age within the aquifer (e.g. Morgenstern, Daughney, et al. (2014)).

Reaction rates can be estimated by averaging, interpolation and/or upscaling of field measurements. For example, the rates of weathering reactions that release phosphorus from minerals in the soil zone have been generalised for different soil types in New Zealand (Parfitt et al. 2008). Virus die-off rates in New Zealand groundwater systems have also been generalised based on available field measurement (Moore et al. 2010).

Reaction rates can also be estimated through contaminant mass balance approaches (Parfitt et al. 2006; Parfitt et al. 2008). In this method, the total contaminant inflows are generally assumed to be equal to the total outflows for the water body of interest, and any imbalance is ascribed to a gain or loss resulting from a reaction that has not been specifically measured. For example, an N balance for all of New Zealand suggests that a total of 3.5×10^7 tonnes of N are removed annually by denitrification from freshwater systems excluding soils (Parfitt et al. 2006).

For more localised and spatially variable estimates, reaction rates can be estimated through the calibration of a groundwater reactive transport model (Parkhurst and Appelo 1999; Xu et al. 2004; Bethke 2007; Parkhurst et al. 2010; Bethke et al. 2021). This approach involves optimisation of the model's adjustable parameters to achieve a good fit between the modelled concentrations and the measurements made at specific sites that are represented within the groundwater model, such as wells, springs, streams. As noted above, this type of groundwater modelling requires specification of the inflows of the contaminant to the groundwater system over time. If these historical inflows are well known, any differences between the measured and modelled concentrations that cannot be explained by conservative (non-reactive) transport of the contaminant can be ascribed to reactions, from which the reaction rates can be estimated.

Finally, reaction rates can be inferred by the contaminant concentrations in groundwater samples to the inferred age distributions of water in those samples derived from model fitting to age tracer data. For instance, concentrations of dissolved phosphate and silica are both found to increase with the mean residence time of water in the Lake Rotorua catchment (Figure 18). These relationships allow calculation of the rates of governing water-rock reactions, which were found to be dependent on rock type for the solubilisation of silica but not for phosphate (Morgenstern, Daughney, et al. 2014). A national-scale study has also been undertaken to provide estimates for water-rock reaction rates for a broader range of New Zealand aquifers (Morgenstern and Daughney 2012).

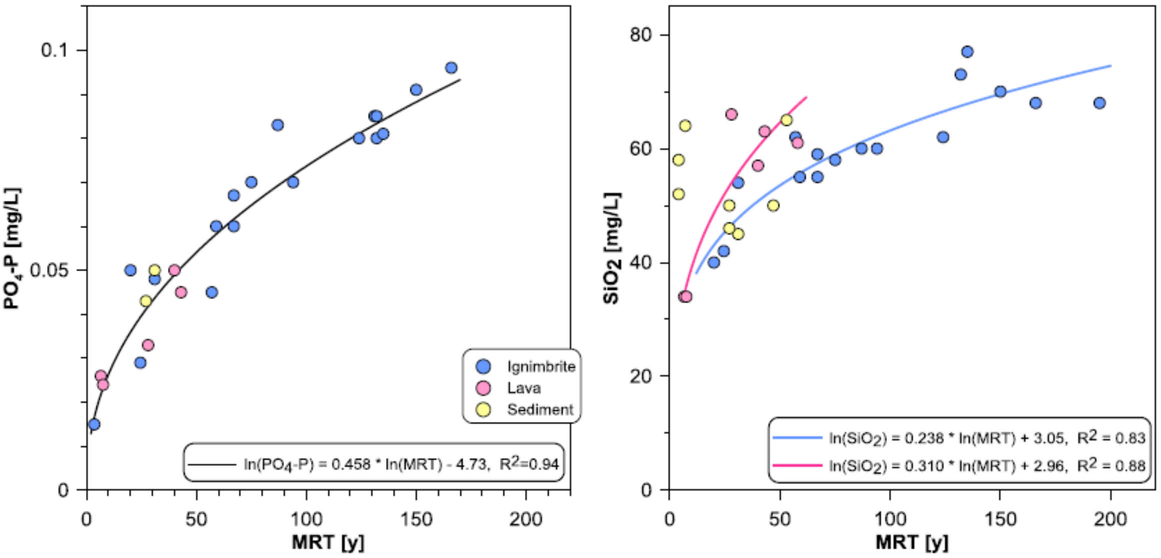

Figure 18: Relationships between mean residence time (MRT) and concentrations of phosphate (left) and silica (right) in the Lake Rotorua catchment. Points represent individual locations from which water samples were collected, colour-coded according to dominant rock type upstream. Source: (Morgenstern, Daughney, et al. 2014).

2.5 Rivers

New Zealand has close to 400,000 km of total river length. The River Environment Classification (REC) categorises the nation's rivers according to climate, geology, land cover and other important characteristics, and represents the river channels in a digital drainage network.

As a key line item in water flow accounts, rivers route and deliver water fluxes from precipitation across the land surface to the sea, often with exchange fluxes with lakes, constructed reservoirs and groundwater along the way (Griffiths et al. 2021). Rivers are, however, often not included as an individual line item in a water stock account because the volume of water they contain is relatively small compared to other compartments of the hydrologic system such as soil moisture or groundwater.

2.5.1 Measurement

River gauging measurements are routinely used to assess flow rates (fluxes of water) at several hundred river flow and/or stage (level) monitoring stations across New Zealand (Figure 19). These stations are operated by regional councils, NIWA and other organisations and typically employ automatic sensors with telemetered delivery of measurements in near real-time, with much of the data freely available to the public (Land Air Water Aotearoa nd; NIWA nd-a). Note that these stations vary in terms of the quality, length and completeness of their historical data (Booker and Woods 2014; Singh S et al. 2019). Furthermore, because many of these stations are operated for flood management or dam/reservoir management, they are not necessarily optimally distributed for water accounting purposes.

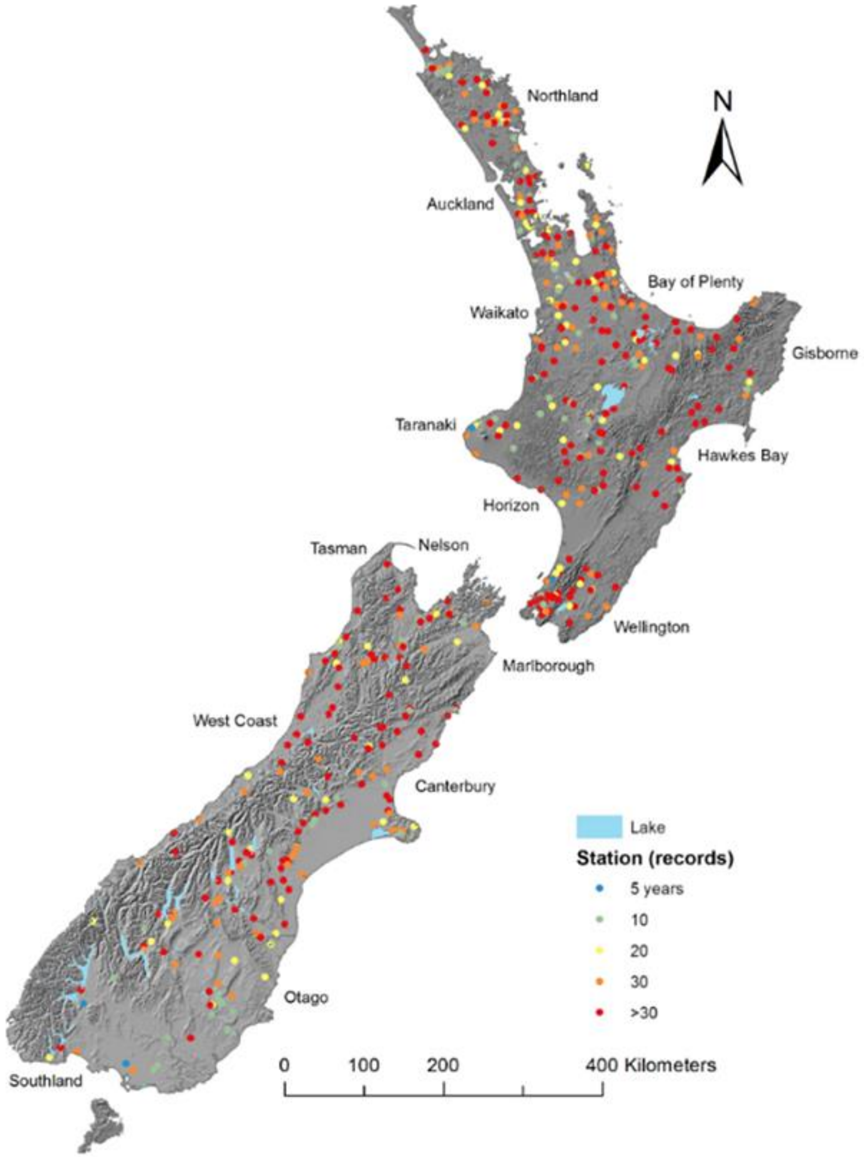

Figure 19: The locations of 482 flow gauging stations considered to have sufficient length and quality of data record for use in a recent national-scale study. Source: (Singh S et al. 2019)

2.5.2 Modelling

A variety of rainfall-runoff models have been developed for New Zealand. These cover the national-, regional- and catchment-scales with varying degrees of spatial and temporal resolution as described below. It is beyond the scope of this report to review and compare each of the available models but, in summary, they collectively represent a range of tools and approaches that can be used to estimate current, past and future river flows for water accounting purposes.

At the national scale, the TopNet model has been developed to simulate the main physical processes in the hydrological system at an hourly time step, including runoff, infiltration, river flow, soil moisture and groundwater level (Figure 20, Bandaragoda et al. (2004)). When uncalibrated, the TopNet model simulates naturalised conditions (Bandaragoda et al. 2004; Booker and Woods 2014), but it can be validated and/or calibrated by comparison to flow measurements and other data to improve its regional- or catchment-scale performance, including representation of human modifications such as abstraction, storage, channelisation, impervious surfaces, etc.

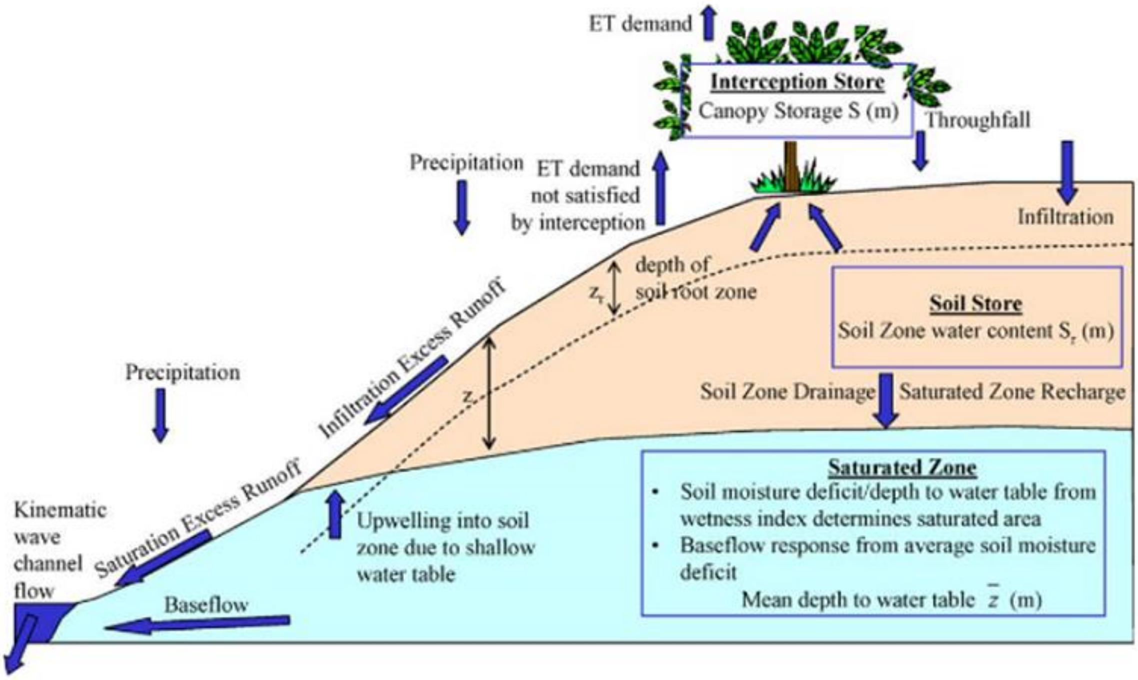

Figure 20: Schematic of the physical processes represented in the TopNet model. Source: (Bandaragoda et al. 2004).

For water accounting purposes, the TopNet model can be used to estimate river flows and flow statistics at places for which measurements are not available (e.g. Singh S et al. (2019) and Booker and Woods (2014)). This can provide national-, regional- and catchment-scale estimation of key descriptors of river flux for any reach over a specific time period (e.g. (NIWA nd-b)).

For example, TopNet is used to estimate the river flux component of the national-scale water physical stock accounts (Griffiths et al. 2021), for which a key line item is the total water outflow to the sea (Figure 21). Model estimations are necessary for this purpose for most rivers because few gauging stations are situated exactly at the coast.

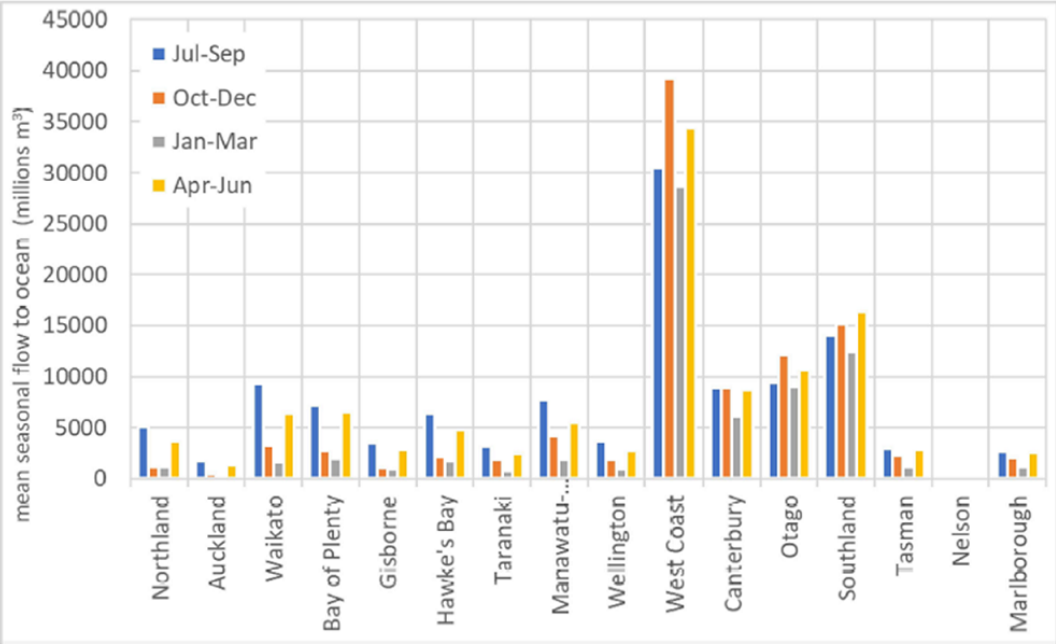

Figure 21: Estimated mean seasonal river flows to the sea by region, 1995-2020. Source: (Griffiths et al. 2021).

Also for water accounting purposes, the TopNet model can be used to hindcast or forecast flows for different time horizons. For short-term river flow predictions, TopNet can be coupled to a weather forecasting model. For example, coupled to the weather forecasts generated by the NZCSM (Section 2.2.2), TopNet is currently generating hourly forecasts of river flows, with 48-hour lead time, for approximately 60,000 river reaches (Strahler 3) across New Zealand. The TopNet model is also being used to produce estimated river flows over longer seasonal and multi-decadal (climate change) time horizons (Figure 22).

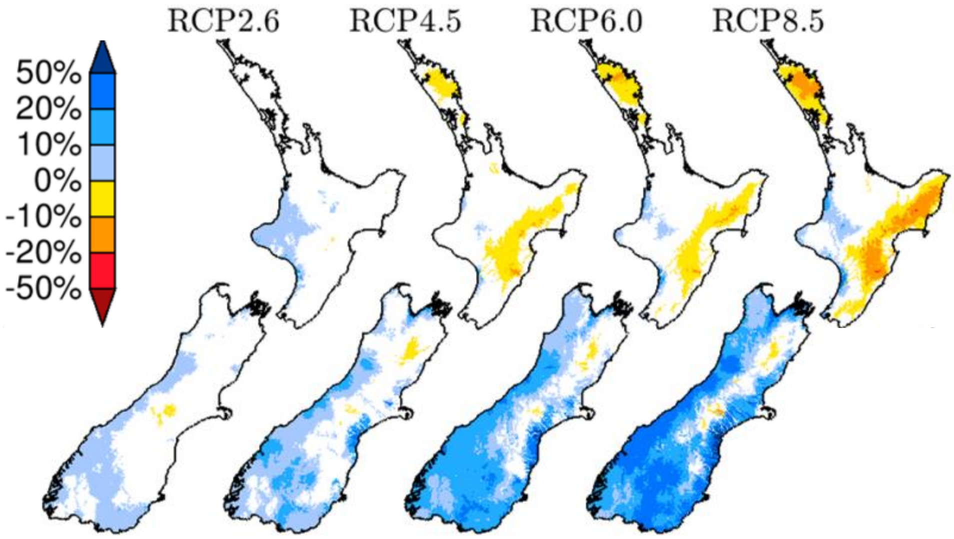

Figure 22: Projected change in mean annual river flow for the period 2080-2099 relative to the reference period 1986-2005 under different RCP emissions scenarios. Source: (Collins D 2020).

While TopNet is the best known national-scale model presently available to estimate river -flows, other physically-based modelling tools have been applied in New Zealand at the national, regional- or catchment-scale, including MIKE-11 (Wallace 2009; Oliver and Wild 2016; DHI Water and Environment Ltd 2020), MIKE-SHE (Durney et al. 2016), eWater SOURCE (Blyth et al. 2018; Easton et al. 2019) and SWAT (Me et al. 2017; Hoang 2019, Parshotam, 2020). These models differ in terms of the physical processes that they include and the spatial and temporal scales at which they can be applied, but all are able to provide estimates of river flows and allow model calibration based on measured data. In addition to these physically-based models, river flows and/or hydrological indices have been estimated using statistical or machine learning methods for some New Zealand catchments (Booker and Woods 2014; Booker et al. 2017).

2.6 Lakes

New Zealand has 3,820 lakes greater than 1 hectare in size (Ministry for the Environment and StatsNZ 2019). The total water stock in New Zealand's lakes has been estimated to be 405 km^2 (Toebes 1972). However, for reasons explained below, due to the challenge of accurately determining the total volume of water stocks in New Zealand's lakes, the national accounts presently only report on the relative change in lake water stocks (Griffiths et al. 2021)

This section discusses lake water flows into/from rivers, whereas lake water flows into/from groundwater are discussed in Section 2.4.1.3.

2.6.1 Measurement

The total stock of water contained by a lake cannot be directly measured but is most straightforwardly estimated from its bathymetry and measured water level. Application of this approach at the national scale is hampered by incomplete coverage of lake level measurements, with lake level data available for only 73 lakes and often with gaps in the historical record (Table 1, Griffiths et al. (2021)) and bathymetry data available for only a subset of New Zealand's lakes (https://niwa.co.nz/publications/charts#lake). In the absence of in-situ lake level measurements, estimates can be made using satellite interferometric radar (Cretaux et al. 2016), though this approach is not common in New Zealand. In the absence of bathymetric survey data, bathymetry can be estimated from lake area and lakeside topography (Heathcote et al. 2015) or volume-area scaling (Cael et al. 2017), but these approaches are also not common in New Zealand and can have large errors. Because of the challenge of determining the total lake water stock in absolute terms, the national accounts instead report on the change in lake water stocks between two reporting periods based on the measured net change in lake water level (Griffiths et al. 2021).

Total lake volume divided by the outflow rate gives the hydraulic residence time which is an important factor in estimation of nutrient attenuation within lakes by burial in the sediment. In view of the difficulty in obtaining lake volume from bathymetry this information is not available for many lakes although it can be approximated from few measurements because lake volume is equal to lake area times mean depth.

Regarding flows through lakes, total inflows to lakes are often best estimated by difference from the remaining components of the water balance because it is often impractical to monitor all surface inflows and the proportion of direct groundwater inputs and its variability are often unknown.

Table 3: Data availability for lakes as reported in the 2020 water physical stock accounts. Level of and range of completeness is provided as the number of lakes for which all of the required information was available in full, and the number of lakes for which the information was only partially available (in brackets). Source: (Griffiths et al. 2021)

Regions	Number of lakes reported in 2020 accounts	Level completeness and range over 1995-2020 [%]	Number of lakes fully and partially (in bracket) reported for 2020
Auckland	11	86.5 [27.5-96.2]	1 (0)
Bay of Plenty	13	91.6 [0-100]	5 (7)
Canterbury	11	94.6 [82.1-100]	3 (3)
Otago	9	98.5 [94.6-100]	6 (3)
West Coast	3	87.1 [82.4-91.4]	1 (1)
Hawkes Bay	1	96.2 [96.2-96.2]	1 (0)
Manawatu	5	50 [0-96.2]	0 (0)
Waikato	13	96.3 [94.9-100]	1 (10)
Wellington	2	48.2 [0-96.5]	0 (1)
Southland	4	99.8 [99.4-100]	4 (0)
Tasman	1	88.2 [88.2-88.2]	0 (0)

2.6.2 Modelling

An alternate to the above-listed methods for estimating change in lake water stocks is to develop a water balance based on itemised inflows and outflows. Each of these itemised terms in the lake water balance must be estimated individually using measurements and/or models as described in other sections of this report. For example, this water balance approach has been applied for Lake Wairarapa, based on measured or estimated monthly precipitation, evapotranspiration, surface water inflows and outflows, abstraction and groundwater seepage, and found to yield comparable estimates for change in total storage as determined from monitored lake levels (Thompson and Mzila 2015). Similar lake water balance calculations have been developed for other New Zealand lakes, including Lake Horowhenua (Thomas and Gibbs 2014), Lake Rotorua (Rutherford et al. 2009; Daughney CJ et al. 2015) and Lake Tarawera (Hamilton et al. 2006).

While more complex than estimating changes in lake water stocks more directly based on measured water levels, the approach of developing an itemised water balance may be appropriate or even required if the lake is treated as a stand-alone IOU for water accounting purposes.

Stocks of contaminants in lakes and constructed storage such as dams can be estimated by simple multiplication of concentrations and water volume. Likewise, flows of contaminants are estimated by multiplication of concentrations and water flow through inlets and outlets. Methods to determine mass balances of nutrients, phosphorus and fixed N for lakes are presented in Verburg et al. (2018). The methods, in part based on methodology first developed by Vollenweider (OECD 1982), are used to estimate total inputs of nutrients to lakes from the catchment and from the atmosphere, losses through the outlet, and removal within the lake either by burial in the sediment or, in the case of fixed nitrogen, by loss to the atmosphere by denitrification. The mass balance equations also provide means to estimate internal loads from the lakebed sediment. The same mass balance methods are generally valid for other contaminants that pass through lakes.

2.7 Wetlands

In many regions, wetlands are an important but complicated “asset” to record in water quantity accounts. Wetlands are an interface between terrestrial and freshwater (and other open water) systems; definitions vary but generally are considered as places where the water table is usually at or near the surface, and/or where land is covered by shallow water permanently or seasonally. They are often but not always associated with riparian areas near water bodies and/or with depressional areas containing water before it reaches water bodies, and areas where significant groundwater reaches the surface or near surface. As many expand and contract significantly seasonally and in response to precipitation events or the lack thereof, it is also difficult to define volumetric or areal spatial boundaries around them. Choices of how to handle boundaries between wetlands and other IOUs are therefore important. If the area/volume is allowed to expand and contract, which may be most suitable for some wetland accounting purposes, it may add additional complexity to accounting for surrounding areas therefore also needing to contract and expand over time. Wetland types are often classified by the origin of their source water: groundwater, precipitation, riverine, or combinations of two or all. These varied sources are characterised by different water chemistry and result in distinctive wetland nutrient cycling patterns. Some are geographically isolated, increasingly we need to consider constructed treatment wetlands, riparian wetlands, bogs, and fens or seeps: all present unique components to consider when calculating their water budgets. As for contaminants, the methods covered in the soils, lakes, groundwater and river sections together generally cover the appropriate methodologies for application to wetlands – the precise mix of which is wetland type-specific.

2.7.1 Measurement

In all types of wetlands, measuring water depth above ground and moisture content below ground is important. Piezometers are used to measure groundwater levels, soil moisture and tensiometers are used to understand water content and suction pressure in shallow not fully saturated soils, and checks on staff gauges or automatic pressure transducers can be used to measure surface water levels. Depending on the sources of water, inflows and outflows from surface water and groundwater sources may also need to be monitored - see the surface water and groundwater sections for details on how to do this. If the wetland is mostly isolated/fed by direct precipitation meteorological stations at the wetland itself will give a more accurate understanding of the water inputs than attempting to extrapolate precipitation and evapotranspiration demand from further away stations.

2.7.2 Modelling

A water balance approach is commonly applied to wetlands, and the significant components vary depending on the type of wetland (isolated, precipitation fed, riparian, surface water fed, or groundwater fed). The approach is similar to that applied to the soil moisture accounting modelling, already described, although it generally lumps together (or treats separately and combines) changes in amounts of open water, soil water, and sometimes some groundwater components within the volumetric or areal element of interest. Complexities arise if the wetland significantly expands and contracts; water balance approaches with changing boundaries are non-trivial and also may impact account calculations in surrounding areas.

2.8 Snow and ice

Measurement (and modelling) of snow and ice is known to be challenging, but there is significant and globally recognised expertise in New Zealand research institutions around these topics and procedures to combine snow modelling, remote sensed snow and ice, and ice mass balance surveys to inform accounts have already been developed to support New Zealand reporting on the SEEA water accounts (Griffiths et al., 2020). In most applications of contaminant accounting, it is not thought likely that snow and ice will be significant contributors of most contaminants of interest, and as long as atmospheric deposition to snow and ice are accounted for, little more detail is likely to be needed.

2.8.1 Measurement

In situ observations of ice mass balance changes typically rely on seasonal snow stake measurements which are expensive and time consuming to undertake each year. It is not practical to undertake wide-spread ground-based snow stake and mass balance measurements for the (admittedly reducing) but still significant areas of ice coverage in the South Island. Nevertheless, there is significant ongoing effort in New Zealand monitoring several key glaciers which provides a useful check on estimates based on remotely sensed observations. Since 1978, oblique aerial photography has also been used on a near-annual basis to capture Southern Alps ice changes by monitoring key index glaciers spread across the Southern Alps. Baumann et al. (2020) recently completed a re-evaluation of the New Zealand glacier inventory using satellite imagery using a Landsat 8 semi-automatic classification method checked against Sentinel-2 MSI data. As of 2016, New Zealand glaciers cover ~794 ± 34 km^2. Only 15 glaciers are located on the North Island, and cover ~3km^2.

2.8.2 Modelling

A relatively novel approach has been recently applied to the Southern Alps to quantify glacier volume change from end of summer survey photos of index glaciers. The method involves using aerial photographs with Structure-from-Motion Photogrammetry (SfM) software to generate 3-D models of the glaciers (Vargo et al. 2017). From the 3-D models, annual digital elevation models (DEMs) of the glaciers are created. By comparing these DEMs between different years the change in ice volume, also known as geodetic mass balance, can be calculated

For the purposes of SEEA water accounting, NIWA provided Stats NZ with the change in quantity of water stored as frozen water (permanent and seasonal snow/ice) derived from NZWaM output.

2.9 Constructed storage

New Zealand has many thousands of dams, most of which are small water supply dams on farms.

In most catchments the influence on water stocks and flows of small on-farm dams will be sufficiently small to ignore. However, in some catchments the cumulative effect of many small dams will be sufficiently large to warrant the inclusion of stored volume in a stock account, and inflow/outflow fluxes in a flows account.

There are more than 400 dams in New Zealand that have storage capacities greater than 18 million litres. They range in height from two metres to 118 metres (the latter height being New Zealand's largest dam, the Benmore Dam on the Waitaki River). Some of these large dams were built to store water for irrigation, others for power generation, and others for domestic and industrial supply or flood water control, and some serve multiple purposes. They must be included in Freshwater Accounts.

2.9.1 Measurement

Large dams are generally not only heavily regulated but are also heavily monitored due to their economic and/or environmental or social purpose. Areas and volumes are well understood and instruments to monitor changing water height levels are generally cost effective and robust.

2.9.2 Modelling

As per the above, it is generally simple to measure changing water stocks and flows in dams or other constructed storages; however modelling around dam takes and discharges can be useful in examining future scenarios, using rules around minimum and maximum levels and permitted takes under varying environmental conditions, user demand etc.

2.10 Abstraction

A common definition of 'water abstraction' refers to the process of taking or extracting water from a natural source (rivers, lakes, groundwater aquifers, etc.) for various uses, from drinking to irrigation, treatment, and industrial applications. Abstraction is distinct from storage, transfer (movement) and use.

2.10.1 Measurement

Regulations on water takes will generally limit both the maximum volumes and rates of take that can be taken by individuals and enterprises annually and will also limit point takes according to various conditions such as environmental flows. Very significant abstractions and transfers in New Zealand are generally well monitored and reported on, while monitoring of smaller but still significant abstractions are generally considered in terms of maximum amount consented rather than actual takes.

MfE report on the maximum volume that can be taken annually, and the maximum rate of take by primary use, primary source, and region for consents that involve consumptive water takes.

Most large transfers are monitored and governed by consents, and actual transfer volumes will be available for regional and national accounts.

2.10.2 Modelling

Many permitted takes are not measured and so must be estimated (modelled) or assumed to be negligible. If the consent information is provided to models, it is reasonably straightforward to apply some simple rules to get an estimate of likely takes. For example, most hydropower schemes and also irrigation schemes have very fixed regulations around cutting takes when river flow drops to a point that ecology may be impacted, and also drinking water schemes may be required to cut any takes when flow rises to a threshold where the sediment carrying capacity of the river system would be likely to cause damage to infrastructure, and these thresholds are easily implemented in "living" models.

At a national scale, Booker and Henderson (2019) present the modelled potential impact of consented freshwater takes (excluding hydropower consents) on natural river flow across New Zealand. The lack of hydropower consent data is not an issue for the accounts; at least for hindcasts, measured hydropower data on actual takes can be provided by the individual companies, who already provide this to Stats NZ for the SEEA water accounts.

2.11 Use

Use is distinct from abstraction, discharge, storage or transfer. Use can be considered as consumptive or non-consumptive but in reality these are end-members in a spectrum that is probably never 100 percent achieved: any 'consumptive' use likely still has some fraction of the water returned to the hydrological system (e.g. irrigation return flows, leaky pipes), and any 'non-consumptive' use likely has some fraction of the water removed from the system (e.g. evaporation from hydro reservoirs)

2.12 Transfer

Transfer is the movement of water between the places of abstraction, discharge, storage, and use. It is an important element in the flow part of the water quantity accounts. For example, this would include inter-region transfers like from Waikato River to Auckland city for bulk water supply, and also for and between hydropower schemes.

For hindcast accounts, data on transfers should generally be available, but for forecasting purposes assumptions on likely transfers under various meteorological and human use scenarios would need to be made concerning future needs for hydro-power generation, flood and drought mitigation, irrigation use, and the like. Some of these needs are a function of future prices for commodities so estimating what they are likely to be is a non-trivial task.

2.13 Discharges

Where takes are non-consumptive, once storage capacity is exceeded discharges will occur which may not be located at the same point the takes occurred. Hydropower schemes and industrial cooling, for example, may take water from points in rivers and discharge them perhaps some kilometres downstream, or divert water into dams or other storage locations which then discharge water to a different spatial location and with a lag relative to non-anthropogenically modified conditions. "Pristine" point discharges such as major springs may also be useful to consider and record in this accounting category, particularly if the source of water feeding the spring is in a different IOU to that in which the spring discharge occurs.

For urban settings, it is assumed that the contribution of point sources to contaminant catchment loads is captured by consent conditions that mandate the sampling and recording of concentrations and discharges. NIWA collates data for contaminants in urban settings (https://urqis.niwa.co.nz/#/report). Together with discharge these data can be used to establish catchment loads that in turn can be converted, if necessary, into mean or median annual concentrations (Gadd et al. 2018). In rural areas, methods are available to assess the contribution to loads for some contaminants from small point sources such as septic systems (Bowes et al. 2014).

No commentary is given on the measurement or modelling of contaminants from natural sources, except to say that: 1) objectives for water quality cannot be set below those under natural conditions, and where natural sources are perceived to cause a water quality issues, there is provision to make an exception for this under the NPS-FM; 2) natural contributions are incorporated into existing measurements and modelling; and 3) if it is necessary to separate the contribution of natural sources from anthropogenic sources, estimates of concentration and loads of contaminants lost from natural sources are available at the reach level for different combinations of climate, topography and geology (McDowell R.W. et al. 2013; Snelder et al. 2018).

2.14 The role of modelling in supporting accounting systems

Some forms of modelling are critical to extrapolate information from the available measurements in space and time. In addition, although one key purpose of the accounts is to track "progress to date" to identify trends, changes, and possible issues with human compliance, there is also an important role for the accounts to support scenario analysis of different futures. As we cannot measure those potential futures until we meet one, far fewer data become available and additional modelling techniques are required to forecast future accounts. Such futures could be projections/forecasts from days to weeks (flood and drought forecasting, hydro-dam storage predictions using forecast models of expected precipitation and evapotranspiration for example), to predictions of what water quality and quantity in a river might look like in decades to hundreds of years given different climate and/or land management scenarios.

Modelling, particularly complex physically-based modelling, does comes with a specific set of challenges around data quality. Such models have inherent uncertainties due to simplifications in their structure but are also generally processing multiple data sources each with their own uncertainty. Validating and having a good grasp on uncertainty in model outputs is essential before relying heavily on them for policy decisions or compliance monitoring.

This section first discusses interpolation/extrapolation methodologies. It briefly notes participatory modelling approaches, which are rarely covered in the hydrological modelling literature but may have a place in water accounting. It then moves to a coverage of more standard hydrological modelling approaches and presents a classification of different types of hydrological models which may be fit for purpose in some water accounting contexts. It then discusses issues around data and model uncertainty, model sensitivity to errors and uncertainty in inputs, and ways to establish degrees of confidence in models (and establish where they may or may not yet be fit for decision support purposes, including use or confidence where they have informed account items in the stock and flow tables).

2.14.1 Spatial interpolation and extrapolation

Spatial interpolation and extrapolation techniques can be used to produce comprehensive maps. In principle, there are two main groupings of interpolation techniques: deterministic and geostatistical.

Deterministic interpolation techniques create surfaces from measured points. A deterministic interpolation can either force the resulting surface to pass through the data values or not. An interpolation technique that predicts a value that is identical to the measured value at a sampled location is labelled an 'exact interpolator'. An inexact interpolator predicts a value that can be different from the measured value; this can be used to avoid sharp peaks or troughs in the output surface. The most basic exact interpolator is called the inverse distance weighted (IDW) interpolation, other exact techniques include radial basis functions which involve different assumptions on the relation between distance and values that can be attributed to points in a landscape.

Geostatistical interpolation techniques rely on statistical algorithms to predict the value of un-sampled pixels based on nearby pixels in combination with other characteristics of the pixel. The most widely used form of geostatistics is kriging, and its different variations. These include ordinary, simple, universal, probability, indicator, and disjunctive kriging. Kriging is divided into two distinct tasks: quantifying the spatial structure of the data and producing a prediction. Quantifying the structure involves fitting a spatial-dependence model to the data. To make a prediction for an unknown value for a specific location, kriging will use the fitted model from variography, the spatial data configuration, and the values of the measured sample points around the prediction location. Because geostatistics is based on statistics, these techniques also produce error or uncertainty surfaces, giving an indication of how good the predictions are – at least in terms of the spatial interpolation errors (note that the values themselves may also be prone to uncertainty).

2.14.2 Participatory / mediated modelling and mapping

Participatory modelling involves engaging with stakeholders to create representations of reality. Such approaches may aid understanding less tangible attributes of water bodies such as non-use values.

Participatory modelling involves co-constructing a model, alongside key stakeholders, and often significantly improves model credibility and helps establish buy in from user groups. Participatory mapping is a similar approach where people are asked to map locations that are important to them for different reasons, Incorporation of these “non-traditional” hydrological modelling approaches may be particularly important for understanding cultural values and connections to entities such as rivers, lakes and springs in the water accounts.

2.14.3 Model-structure based classification(s)

There are a variety of ways to classify hydrological models, we follow here the popular classification system presented in Wheater et al. (1993) and further described in Pechlivanidis et al. (2011); where models are classified based on their model structure, spatial distribution, stochasticity, and spatial-temporal application.

In terms of structure, at a high level, models (or sub-models) can be divided into three distinct classes: empirical (called “metric” by Wheater et al), conceptual and physics-based. The essential characteristic of empirical models is that they are primarily based on observations and seek to characterise the system response from the available data (Wheater et al. 1993). Their reliability in a given application depends on the range of available input and output data. They often perform very well and efficiently when applied in similar contexts and conditions to which the model was developed and initially calibrated, but are more dangerous when extrapolated to extreme events or ungauged catchments. Interesting developments may be coming for models of this type with the increasing advances in machine learning (or artificial intelligence) over recent years. Supervised machine learning, where some process constraints or thresholds can be imposed, are being developed and tested for a large variety of complex modelling exercises including modelling hydrological services. Well-known examples of machine learning algorithms are random forest and CNN convolutional neural network (CNN). Spatial patterns can be included in the analysis, for instance the coordinates of each pixel or distance to a riverbed may be included in the dataset of independent variables.

Conceptual models generally represent in a simplified form the main component hydrological processes perceived to be of importance in catchment scale input-output relationships. This type of model varies considerably in complexity and the model structure tends to be based on extensive use of schematic storages, which are combined to represent a conceptual view of the important hydrological features. Models can vary in complexity from two or three simple storages up to a highly complex representation. As they generally are designed to consider key processes and thresholds (to the extent we understand them) they have some advantages over empirical models when transferred for use in geoclimatic or other conditions they were not calibrated to, and to ungauged areas, but not all of the model parameters have a direct physical interpretation (i.e. they are not independently measurable), so have to be estimated through calibration against observed data.

Physic-based models represent the component hydrological processes such as evapotranspiration, infiltration, overflow, and saturated and unsaturated zone flow using the governing equations of motion (usually formulated as non-linear partial differential equations) based on continuum mechanics. Generally, the equations of motion of the constituent processes are solved numerically using a finite difference, finite element or finite volume spatial discretization. In theory, physics-based models are defined by wholly measurable parameters and can provide continuous simulation of the runoff response without calibration, but this is never fully true in hydrological modelling applications. The physics behind the model structure are generally based on laboratory or small-scale in-situ field experiments, and hence are affected by the nature of the experiments themselves. Extrapolation to larger (e.g. catchment) scales often involves the assumption that the physical processes and properties are independent of scale, raising uncertainty about their applicability. Catchments typically have a high level of spatial heterogeneity which can be prohibitively expensive to observe or comprehensively represent in the model. This is most obvious in the representation of subsurface processes because of the difficulty of observation and the high degree of soil/aquifer heterogeneity which often exists. To reduce computational burden and data requirements, simplified physics/mechanics are sometimes used to represent the physics (e.g. simplified St. Venant equations and the Green-Ampt equation), leading to deviation from the physical basis and additional questionability.

Many models are labelled as one of the above types but in truth include elements of two or more. Hybrid metric-conceptual models have been developed to combine the strengths of data-based and conceptual models. Many so-called physics-based models are in fact hybrid physically-based-conceptual models (e.g. SWAT (Arnold et al. 1993)). These aim to simplify model structure by representing some of the mathematical-physics based processes in a conceptual manner, particularly in cases where physical parameters are difficult to measure. In principle this may lead to some improvement in parameter identifiability, although such models often still have very high dimensionality of the parameter space.

2.14.3.1 Lumped and distributed models

Lumped models treat the catchment as a single unit, with state variables that represent averages over the catchment area. In general a lumped model is expressed by differential or empirical algebraic equations, taking no account of spatial variability of processes, inputs, boundary conditions and system (catchment) geometric characteristics (Sorooshian and Gupta 1995). Distributed models make predictions that are distributed in space, with state variables that represent local averages, by discretising the catchment into a large number of elements and solving equations associated with each individual element. Distributed models take into account spatial variability in processes, inputs, boundary conditions, and catchment characteristics. However, most distributed models use average variables and parameters at element or grid scales, and often parameters are averaged over many grid squares due to lack of data availability. Semi-distributed models have been suggested to combine the advantages of both types of spatial representation. This type of model does not pretend to represent a spatially continuous distribution of state variables; rather it discretises the catchment to a degree thought to be useful by the modeller using a set of connected and interacting lumped models. A semi-distributed model can therefore represent the important features of catchment, while at the same time requiring less data and lower computational costs than distributed models.

2.14.3.2 Deterministic and stochastic models

Models can be classified as deterministic when the results are uniquely determined through known relationships between the states and data. Deterministic models produce a single result from a simulation with a single set of input data and parameter values, and a given input will always produce the same output, if the parameter values are kept constant. Stochastic models use random variables to represent process uncertainty and generate different results from one set of input data and parameter values when they run under "externally seen" identical conditions. A particular set of inputs will produce an output according to a statistical distribution. This allows some randomness or uncertainty in the possible outcome due to uncertainty in input variables, boundary conditions or model parameters. Mixed deterministic-stochastic models can also be created by introducing stochastic error models to the deterministic model. There are many advantages to the incorporation of some degree of stochasticity for many modelling purposes, but we warn that for replicability in the accounts, particularly as they are developed and tested, the changing parameters associated with any stochasticity in the models should be saved along with the model outputs so results can be regenerated as necessary.

2.14.3.3 Time and spatial scale based classifications

Regarding time, some classification systems distinguish between event-based models and continuous models – the former designed to model single, generally significant rainfall events, the latter multiple events and input-output relationships over longer time-frames. We focus here on continuous modelling as event-based models are not likely to be particularly relevant to water accounting. The time scale may be defined by the time intervals used for input and internal computations, or by those used for output and calibration of the model, and the choice is usually a function of the model's intended use. Common classifications of "continuous" time based models are sub-daily, daily, monthly, and yearly.

Considering space, there are a divergence of views in the literature. Some researchers consider models should be classified according to the size of the catchment they can represent: small, medium and large (common breakpoints being 50-100 km^2 between small and medium, 500-1000 km^2 between medium and large). Others base classification on homogeneity, for example the scale at which processes can reasonably be averaged, i.e. the "hydrological response unit" size, or on the level of spatial discretization in the model itself.

2.14.4 Calibration of hydrological models

Model calibration is the process of selecting suitable values of model parameters such that the hydrological behaviour of the catchment can be simulated closely (Wagener et al. 2004; Moore and Doherty 2005). There are two types of model parameters in most models: physical parameters, and process parameters (Sorooshian and Gupta, 1995). Physical parameters represent the physical properties of the catchment and are usually measurable or at least relatable to measurements, such as the catchment area, surface slope etc. Process parameters represent catchment characteristics that cannot normally be measured such as the average depth of water storage capacity, coefficient of nonlinearity controlling discharge rates from component stores, etc (Sorooshian and Gupta 1995). There are some physical parameters, such as the hydraulic conductivity and porosity, which are measurable in theory but difficult to measure in practice, and hence are often calibrated. The calibration process can be either manual or automatic; however in practice is often a combination of the two.

2.14.4.1 Manual calibration

This is a process that mainly depends on the modeller adjusting "by hand" model parameter values until the output of the model closely matches the observed data. The adjustment of the parameter values is made by the modeller by a trial and error process, so familiarity with the model structure and the study catchments saves time and effort. In general, it is difficult to determine the "best fit" or to determine a clear point indicating the end of the calibration process, and hence different results will be obtained by different modellers; a level of subjectivity is always present. The time consuming nature is another problem with this type of calibration.

2.14.4.2 Automatic calibration

The development of computer-based methods for automatic calibration of hydrological models has been partly motivated by the need to speed up (in terms of computational efficiency) the process of calibration. The automatic process can provide more objectivity and reduce the need for expertise with the particular model. However, automatic calibration methods have not yet matured to the point that they can entirely replace manual methods due to the difficulty of constructing objective functions and optimisation algorithms (which replicate human judgement; and hence automatic calibration is often most successful when used in conjunction with a manual procedure).

A typical automatic parameter estimation procedure consists of four major elements: the selected objective function (or performance measure), the optimisation algorithm, the termination criteria, and the calibration data. The objective function (or goodness of fit) is a numerical measure of the difference between the model simulated output and the observed (measured) catchment output (Schaefli and Gupta 2007). Many different objective functions can be found in the literature; however the most common objective functions are based on the standard *least squares methods* (and equivalent methods) and *maximum likelihood methods*. Common least squared statistics include the root mean square error (RSME), the coefficient of determination (r^2) and Nash Sutcliffe Efficiency (NSE). The RMSE is the root mean squared difference between value predicted by the model and observations, the r^2 indicates the proportion of the variance in predictions that can be explained by observations, and the NSE indicates how well a plot of predicted versus observed values fits a 1 to 1 line. Values of r^2 and NSE > 0.75 generally indicate a reasonably good fit between predicted and observed values and hence can be used to give comfort in repeatability or precision of estimates. Values for RMSE should be as low as possible but are dependent on the range in values.

A very important consideration for water accounting is that generally, results based on single objective functions (such as NSE) are biased to individual aspects of the hydrograph. If the objective function for a pre-calibrated model has been selected for a specific modelling task such as flood or drought forecasting, irrigation scheduling etc, it may not be suitable for the purpose of accounting for stocks and flows over broader time scales and/or over more general conditions. There are multi-objective approaches which can consider different aspects of model performance simultaneously, but some aspects of uncertainty exploration and calibration still require multiple objectives to be collapsed into a single point for certain purposes. One common approach is to aggregate the multi-objectives into a single objective criterion and optimise to the single-valued best fit. The result is then strongly dependent on the aggregation, or weighting of the objectives. An alternative is to employ the concept of Pareto optimality, in which a *Pareto set* of solutions is generated with the characteristic that moving from one solution to another results in the improvement of one criterion while not causing deterioration in one or more others.

2.14.4.3 Optimisation algorithms

The surface described by the objective function in the parameter space is called the *response surface*. The optimisation algorithm searches the response surface for the parameter values that optimise (minimise or maximise) the numerical value of the objective function, constrained to the pre-defined allowable ranges of the parameters. Most optimisation methods or strategies can be classified as either *local search methods* or *global search methods*. *Local search methods* are designed to efficiently find the local minimum (or maximum) of a response surface (or over some small neighbourhood). These type of methods seek to continuously proceed in the direction of improving function value to eventually arrive at the location of the function optimum, irrespective of where in the parameter space the search procedure started. Using a local search, we assume that the solution exists at the first point in the response surface where the slope is found to be zero within some specified tolerance, minimising (or maximising) the objective function value. However, recognising that there may be multiple points with near-zero slopes, this is not normally alone an adequate criterion. Hence *global search methods* explore the entire feasible region of the parameter space attempting to find the bottom of the deepest valley. There are three main ways to terminate the search: objective function convergence, parameter convergence, and maximum number of iterations. Based on the function convergence criterion the iterations are terminated when the function value cannot be significantly further improved.

2.14.4.4 Verification

Verification (also known as validation) takes place after calibration to test if the model performs well on a portion of data, which was not used in calibration. Model verification aims to validate the model's robustness and ability to describe the catchment's hydrological response, and further detect any biases in the calibrated parameters (Gupta et al. 2005). Model performance is usually better during calibration than verification period, a phenomenon called *model divergence.* When the degree of divergence is considered unacceptable, the modeller has to examine the model structure, input data and the calibration procedure for valid or inappropriate assumptions or inputs and then revise accordingly.

2.14.4.5 Model sensitivity and uncertainty estimation

As discussed earlier, understanding the uncertainty inherent in model predictions is critical before results can be considered suitable to support policy, management change and/or compliance monitoring. A starting approach is to qualitatively describe all known sources of uncertainty, and ensure this is considered alongside any analysis and decisions.

A better understanding of model sensitivity to unknown parameters and uncertain or erroneous input data can be obtained by performing a sensitivity analysis, where the influence of changes in input data sets and parameters on model output are investigated. Sensitivity analysis evaluates the impact of changes in the model parameters, inputs or (initial) states on the model output of interest. Sensitivity analysis can determine if there is dependence among parameters, if two or more parameters are simultaneously changed. As with automated calibration, there are two types of sensitivity analysis: local sensitivity analysis and global sensitivity analysis. The former type of analysis aims to assess the impact of change in the parameter values within the local region of indifference on the model output. The local nature of this type of sensitivity analysis inherently limits its ability to identify all potentially relevant features of the response surface. However, local sensitivity analysis methods are useful when interested in the local region of indifference while saving computational effort. Alternatively, global sensitivity analysis attempts to explore the full parameter space within predefined feasible parameter ranges. A statistic is used to measure the general variability of the objective function over the space, or a sub-dimension of the space.

Where computational resources permit and there is a reasonable understanding of the distributions of uncertainty associated with input data and parameters, a fuller more formal uncertainty analysis examining the likely distribution of uncertainty in model outputs can be carried out.

Estimating the total uncertainty inherent to a hydrological model involves the identification and quantification of four sources: natural uncertainties, data uncertainties, model parameter uncertainties, and model structure uncertainties. Once these are quantified, there are numerous methods for assessing uncertainty in hydrological models. These can fall into one of three categories: *analytical methods*, *computer algebra based (black box) methods*, and *sampling-based methods*.

Analytical methods involve either the differentiation of model equations and solution of a set of auxiliary sensitivity equations, or the reformulation of the original model using stochastic algebraic/differential equations. Although analytical techniques are computationally efficient, severe assumptions are required as well as access to the underlying model equations and formulation. Therefore they are not generally considered applicable for complex hydrological models.

The most commonly used methods for uncertainty estimation are sampling based strategies which require no access to model equations or even the model code, and only require the model outputs associated to a set of input/parameter combinations. Uncertainty is performed by executing the model repeatedly for sets of parameter values sampled from a probability distribution; however, these methods are computationally expensive.

Monte Carlo (MC) simulation is an extremely flexible and robust sampling-based method widely used for uncertainty problems in hydrological applications. The uncertain parameters are described by probability distributions, and in the absence of information on joint probabilities, model parameters are assumed independent. Random values of each of the uncertain parameters are generated according to their respective probability distributions and the model is run using each random sample. Thereby, samples of model outputs are generated giving statistics (e.g. mean, standard deviation, skewness) and estimated probability distribution of the model output can be determined.

The main disadvantage of MC methods is that a great number of model runs are often required to reliably represent all probable results (and adequately describe the response surface), especially when there are a number of random variables. Although the adequate number of samples is case specific, in general the greater the number of parameters and the greater the complexity of the response surface, the greater the number of simulations that are required. Replication of MC sampling is useful to check convergence.

A degree of computational efficiency can be accomplished using efficient sampling methods which may include heuristic search procedures, or less informed approaches where segments of the probability distributions are split or stratified, and systematically explored. For example, the stratified Latin Hypercube sampling method (Helton and Davis, 2003) divides the range of probable values for each parameter into ordered segments of equal probability and combines the individual samples to produce the parameter sets.

A range of heuristically guided global optimization methods exist, for example algorithms based on genetic evolution principles and Markov Chain Monte Carlo (MCMC) techniques. MCMC methods draw samples from probability distributions based on constructing a Markov chain that has the desired distribution as its equilibrium distribution (Vrugt et al. 2009). Each state is visited the required number of times to satisfy the conditional distribution of the parameters given the data and this is achieved through satisfying appropriate conditions of reversibility (detailed balance) and ergodicity (Hastings 1970). A challenge in MCMC methods is to determine how many steps are needed to converge to the stationary distribution within an acceptable error.

2.14.4.6 Concluding comments on the importance of recognising model uncertainty

The presence of uncertainty should be clearly recognised and considered in any accounting process, particularly where local scale policy decisions may draw on information from the accounts or the models used in their generation. A first check is sensibility, that the model is being applied in appropriate conditions for the context the model has been developed and tested in and that output results look physically and otherwise realistic; and sensitivity and uncertainty analysis are strongly encouraged to understand the range of uncertainty surrounding output predictions. In addition to modelling uncertainty, an important, and sometimes greater, source of uncertainty comes from either the users or quality of the data inputs (Shepherd et al. 2013). These sources of uncertainty are not discussed as they are assumed to be minimised by users' adhering to input data standards.

Where models are highly sensitive to uncertain inputs or their output uncertainties are large, outputs can be translated into forms that users are more likely to recognise are uncertain. For example, risk indices have been used to estimate and communicate the likely magnitude of N, phosphorus, and sediment losses from land to water in New Zealand (McDowell R. W. et al. 2005; Fonterra Co-op Ltd 2020). The phosphorus loss estimate in OVERSEER is listed as a risk of loss owing to a recognition that farm blocks are more often defined and designed to capture nitrogen management than phosphorus management. A focus on N management can result in poor predictions of phosphorus loss if critical source areas of phosphorus loss are not captured. However, when blocked to correctly capture critical source areas, phosphorus loss estimates perform as well as nitrogen loss estimates (r^2 and NSE > 0.7). Internationally, risk indices are used in regulation. For example, in the US, schedule 319 grants for land management actions make use of risk indices to set baselines and measure the effect of mitigation actions (McDowell R.W. et al. 2016). These indices are calibrated against either observed losses or models known to accurately predict losses (see Fig. 23).

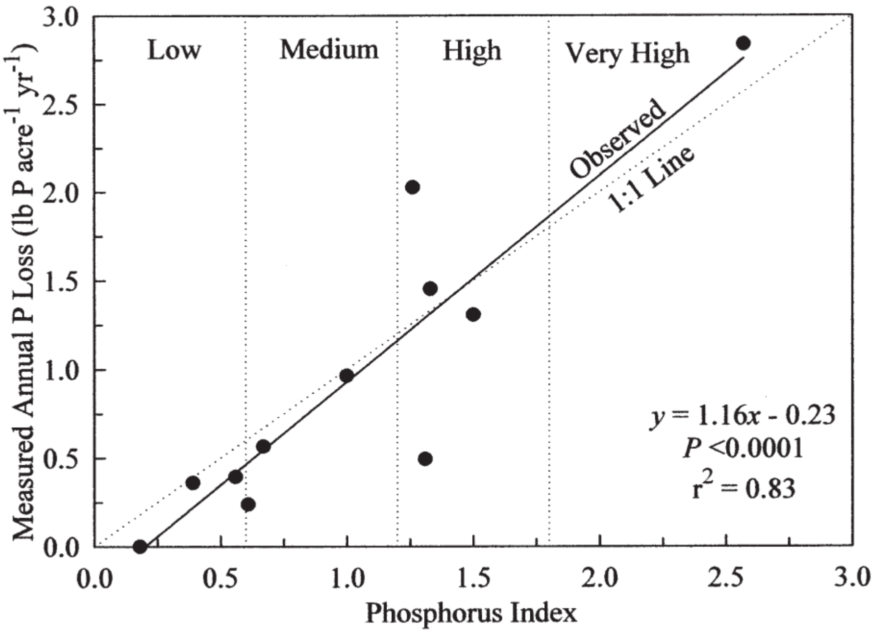

Figure 23: Plot of observed (viz. measured from 0.4 ha catchments) versus predicted values for the Arkansas P index used in regulation to direct farm actions to mitigate P losses 49

A common approach to the management of uncertainty, especially at the land-water interface, where it can have a significant impact on farm management decisions is to: 1) clarify assumptions used in the measurement and modelling of contaminant stocks and flow, which includes communicating the level of uncertainty; 2) recognise that contaminant stocks and flows will vary naturally, but may be compounded by management decisions; and 3) recognise that while observations may relate directly to the freshwater objective, there is likely to be greater uncertainty in modelled predictions – necessitating the use of multiple lines of evidence to support change.

Although it can be easy to say that regional councils have a disparate approach to limit setting and management at the property scale (Maseyk et al. 2018), it is equally valid to say that there is a good degree of standardisation in how councils have adopted the three points above. A good example lies in the lessons learnt in implementing farm practice change at the property level through a combination of measurements and models (like OVERSEER (Freeman et al. 2016)). These lessons apply to any model used at the land-water interface, and are:

- It is recognised that models can only be used in certain land use by climate by management permutations and that other models may be necessary to account for different flow paths or contaminant forms.
- Predictions may change as models are updated. Many councils therefore only advocate the use of models in a relative sense, although some have also stipulated specific version numbers and therefore are left with using outdated versions.
- Natural variation dictates that a single annual prediction is likely to be highly uncertain. Therefore, many councils advocate that a rolling average will give a better estimate of long-term losses.
- If the uncertainties in modelled estimates are known both within and between versions, estimates can be used to judge relative change, i.e., a direction of travel which recognises that while uncertain, there is confidence that actions taken because of modelling will lead to a reduction in contaminant loss.
- If some management practices are likely to have a large impact on contaminant losses, resource consents could be short-term to allow for a fast reassessment of those practices on contaminant losses.
- Some sources of uncertainty can be buffered by using multiple models but there is also increasing recognition that their outputs are best used to meet freshwater objectives when included as part of FEPs which gather other data to create an action plan of practices to mitigate contaminant losses.
- Recognising that while evidence of action is best supported by monitoring, reductions attributable to actions is likely to be diluted by changes that occur beyond the land-water interface (e.g. loss processes such as denitrification (Rivas et al. 2017) and in-stream processing (McDowell Richard W. et al. 2020)). These changes are accounted for by modelling at larger scales (and IOUs) but also by changes in the monitoring network to better detect actions (e.g., shifting or including more monitoring sites closer to sites where actions are occurring).

3 APPENDIX C: UNBUNDLED CONSENTS – AN EXAMPLE

The main suggested change from the consent design and database structures in use in 2013 is the unbundling of the consent to “take and use water” into an Allocation Consent, a Water Take Structure Consent, and a Water Use Consent, each of which serves a different purpose as summarised below.

- The primary purpose of the Allocation Consent is to manage the cumulative effects of all water taken from a water body and provide fair access to the water made available for taking. The scope of the conditions in an allocation consent is limited to these matters. Allocations to individuals should be recorded as time-series, with a time-step of between one day and one year. The time-step needs to match the frequency with which allocations may change.
- The primary purpose of the Water Take Structure Consent is to manage the localised (near-field) effects on the water source and other water takes of the operation of a surface water intake structure or a groundwater bore, and to apply conditions such as requiring water metering on all takes and fish screens on river intakes. The scope of the conditions in the take structure consent is limited to these site-specific matters. Changes to these site-specific consents are not likely to be required very often and can be achieved through existing consent variation processes. This consent is structure specific. Each structure consent is linked to a water body and the consent holder’s allocation consent for that water body. The sum of all water taken from a water body by a consent holder via one or more structure consents must not exceed the sum of the current allocation from the relevant water body for the consent holder and the designated discharge (if any).
- The primary purposes of the Water Use Consent are to manage the effects of using water, such as increasing drainage, and to apply the ‘reasonable and efficient use’ requirement of the RMA. The scope of the conditions in the water use consent is limited to these matters. Changes to these property-specific consents are not likely to be required very often and can be achieved through existing consent variation processes. This consent is property specific. It is linked to one or more water take structure consents and/or contracts with a water supplying entity. These supply the water that is used.

A person who wishes to take and use water must hold one water allocation consent for each water body, such as aquifer or river, from which water is to be taken, regardless of how many water take structures are used to abstract water from a water body. They must also hold a water use consent.

Figure 24 below illustrates the consents that would need to be held for a farm to irrigate. In this example the irrigation water is supplied via three water take structures and a contracted supply from an irrigation scheme. Water Take Structure 3 takes water from a river source under Water Allocation Consent 2 and a designated discharge (a third party discharges water from storage into the river for subsequent taking via Water Take Structure 3).

The allocation limit is specific to the person holding the consent and is that person’s share of the total allocation limit for the water body. It is stored as a time-series. In Figure 24 below, Water Allocation Consent 1 is from an aquifer and Water Allocation Consent 2 is from a river.

Take Structure 3 may take naturally available water up to the limit set under Water Allocation Consent 2 and from water flow specifically discharged upstream for Take Structure 3’s benefit. To test the compliance of Take Structure 3’s operation, the rate of water take from Take Structure 3 is compared to the sum of Water Allocation Consent 2’s allocation limit and the Designated Discharge Consent allocation limit.

Separating the consenting of water allocation from the consenting of water take structures simplifies adding or removing take structure consents, and the operation of intake structures under time-varying water allocations (e.g. as restrictions come into effect).

Each water take structure consent contains the unique ID of the water allocation consent it is linked to.

Each water take structure consent also contains the unique ID of the water use consent it is linked to. If a property is supplied with water from a water supply scheme, that supply is recorded the same way as a water take structure is. Testing for compliance with the Water Use Consent (reasonable use limit) involves comparing this limit with the sum of water taken via consented water take structures and supplied via infrastructure, minus the change in the volume of on-property water storage.

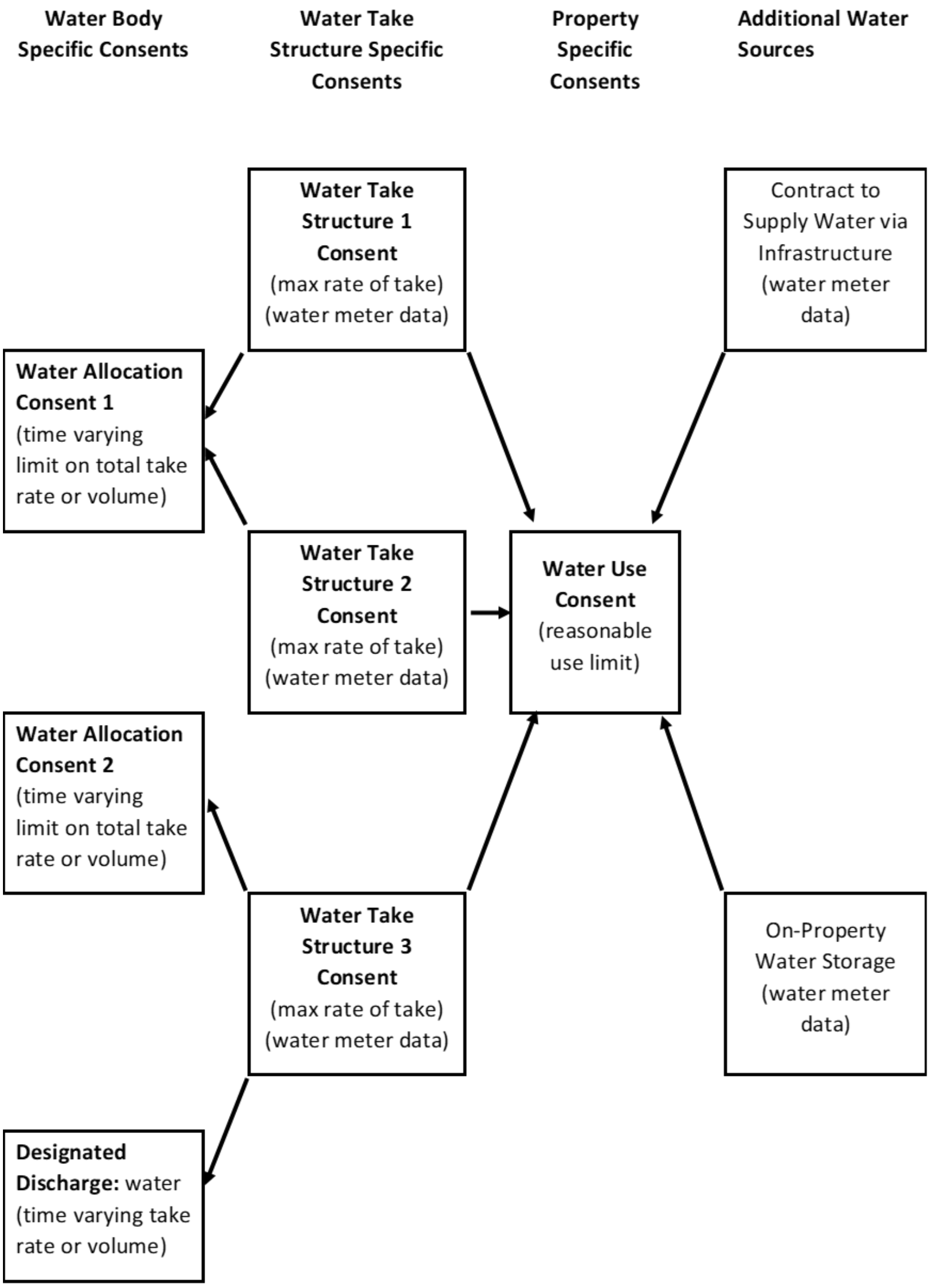

Figure 24: Example of consents needed to take and use water for irrigation. The direction of the arrows indicates the direction of data flow for the purposes of determining compliance with water allocation limits and water use limits.

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