

Analysis of temporal trends in New Zealand's groundwater quality based on data from the National Groundwater Monitoring Programme

C. J. Daughney¹ and R. R. Reeves²

¹ *GNS Science, PO Box 30368, Lower Hutt, New Zealand. Corresponding author: C.Daughney@gns.cri.nz*

² *GNS Science, Private Bag 2000, Taupo, New Zealand*

Abstract

New Zealand's National Groundwater Monitoring Programme (NGMP) aims to provide a national perspective on groundwater quality, and to identify spatial and temporal trends in groundwater chemistry. In this investigation we assessed temporal trends in water quality at each NGMP site using the seasonal Mann-Kendall test and the seasonal Kendall Sen slope estimator. Hierarchical cluster analysis was conducted using the seasonal Kendall Sen slope estimator rates of change of 15 analytes from 108 NGMP sites, in order to define a set of categories representing distinct patterns of trends in groundwater quality that may be associated with specific causes. Cluster analysis revealed five trend-based clusters, with temporal patterns in groundwater quality that appear to relate to either natural water-rock interaction or human influence. The latter are possibly associated with changes in pumping regime and/or changes in land use in the groundwater recharge zone. Assignment of any monitoring site to one of the trend-based clusters defined in this investigation can provide a simple means of summarising temporal trends in water quality.

Keywords

Groundwater, water quality, trend, cluster analysis, baseline

Introduction

New Zealand's National Groundwater Monitoring Programme (NGMP) was established by the Groundwater Group of the Department of Scientific and Industrial Research in 1990. Initially, the NGMP involved only two regions (Tasman and Bay of Plenty). Hawke's Bay and Taranaki joined the NGMP in 1992, Waikato and Manawatu-Wanganui joined in 1994, Canterbury and Wellington joined in 1995, Otago, Northland, Gisborne and Auckland joined in 1996, and West Coast, Marlborough and Southland joined in 1998. The NGMP was designated as a Nationally Significant Database in 1996 by the Foundation for Research, Science and Technology. Presently the NGMP includes 115 sites and is run by GNS Science in collaboration with the 15 regional authorities listed above.

The NGMP aims to provide a national perspective on groundwater quality, and to identify and interpret spatial and temporal trends in groundwater chemistry. Pressures on New Zealand's aquifers are increasing (Parliamentary Commissioner for the Environment, 2004), and thus analysis of changes over time in groundwater quality is important for effective resource management. Analysis of time series data allows for early detection of degrading groundwater quality, for differentiation of short-term fluctuations

Table 1 – General characteristics of hydrochemical facies in the NGMP based on median values of selected water quality parameters (after Daughney and Reeves, 2005)

1	Surface-dominated Oxidised Unconfined aquifer Low to moderate TDS ¹ Ca-Na-Mg-HCO ₃ water	1A	Signs of human impact Rainfall recharge? Moderate TDS Na-Ca-Mg-HCO ₃ -Cl water	1A-1	Moderate human impact Carbonate or clastic aquifer Ca-Na-Mg-HCO ₃ -Cl water
		1B	Little human impact River recharge? Low TDS Ca-Na-HCO ₃ water	1B-1	Carbonate or clastic aquifer Ca-HCO ₃ water
	Groundwater-dominated Reduced Higher TDS Ca-Na-HCO ₃ water			1B-2	Volcanic or volcanoclastic aquifer Na-Ca-Mg-HCO ₃ -Cl
				2A	Moderately reduced Majority unconfined High TDS
2				2B	Highly reduced Majority confined Highest TDS

¹ Total Dissolved Solids

from long-term trends, and for differentiation of changes in water quality arising from anthropogenic as opposed to natural causes.

This paper provides a summary and analysis of temporal trends in New Zealand's groundwater quality, based on data collected through the NGMP. In this investigation, a trend is defined simply as a monotonic change in a data series that is evident over several years (Helsel and Hirsch, 1992). Our aims are to update previous articles on temporal trends in the nation's groundwater quality (Rosen, 1999) and to provide resource managers with a means of comparing data from the NGMP to data from regional council groundwater quality monitoring programmes.

A major objective of this communication is to identify patterns of change amongst several different water quality parameters through the use of multivariate statistical methods. Here we use hierarchical cluster analysis and other complimentary statistical methods to define a set of categories representing patterns of change in groundwater quality over time

that may be associated with specific causes. Daughney and Reeves (2005) recently used a similar approach to define six hydrochemical facies for New Zealand's groundwaters, based on the median values of selected water quality parameters (Tables 1 and 2). Median values of certain water quality parameters have also been employed to categorise New Zealand's rivers (Close and Davies-Colley, 1990) and for classification of groundwaters in other countries (Frapporti *et al.*, 1993; Güler *et al.*, 2002). However, to our knowledge, the hierarchical cluster analysis approach has never been applied to a national-scale categorisation of groundwaters based on temporal trends in water quality.

A second major objective of this investigation is to define baseline (i.e., 'normal') rates of change in groundwater quality at the national scale. The term 'baseline' is typically used interchangeably with the term 'background' in the environmental sciences to describe the natural characteristics of systems in the absence of human influence.

Table 2 – Analyte concentrations (g m^{-3}) at centroids of hydrochemical facies defined by Daughney and Reeves (2005)

Analyte	1A-1	1A-2	1B-1	1B-2	2A	2B
Br	0.07	0.1	0.02	0.04	0.07	0.2
Ca	15.5	13.1	18.7	6.4	26	57.6
Cl	16.9	24.7	3.1	7.3	18	46.3
F	0.07	0.03	0.07	0.04	0.13	0.21
Fe	0.01	0.02	0.01	0.02	0.22	1.25
HCO ₃	69.7	51.3	70.6	34.2	153	345
K	1.36	3.1	1.06	1.46	2.36	5.91
Mg	7.1	7.8	2.7	2.3	7.5	13.3
Mn	0.01	0	0	0	0.07	0.44
Na	15.6	20.8	5.6	8.4	26.8	60.3
NH ₄ -N	0.01	0.01	0	0.02	0.15	0.92
NO ₃ -N	1.51	4.68	0.62	0.73	0.02	0
PO ₄ -P	0	0.02	0	0.02	0.03	0.05
SiO ₂	19.2	47	11.7	23	27.6	38.4
SO ₄	11.6	8.6	5.2	3.9	5.8	0.3
TDS ¹	158.6	181.4	119.4	87.7	269.3	581.5

¹ Total Dissolved Solids (calculated by summation)

The definition of baseline at the national or regional scale provides a general but powerful comparative tool: a site cannot be defined as 'affected' or 'abnormal' unless the threshold limit of normality (baseline) has been previously defined. Baselines must be defined as ranges of values rather than as single numbers, due to the range of conditions encountered in natural systems. In groundwater, for example, the concentration of any parameter may depend on variables such as aquifer lithology, aquifer confinement, geographic area, recharge source and groundwater age. To account for this natural variation, several previous studies have defined baseline for various analytes in groundwater based on arbitrarily chosen percentiles (e.g., 25th and 75th or 5th and 95th) (Newcomb and Rimstidt, 2002; Lee and Helsel, 2005; Daughney and Reeves, 2005). In this investigation, we employ the same approach to define baseline for rates of change in hydrochemistry in New Zealand's groundwaters, which, to our knowledge, has not been attempted in any previous investigation.

Methods

Data collection and screening

At the time of writing (December 2005), the NGMP included 115 sites across New Zealand. To utilise the maximum amount of data for statistical interpretation, we also include 38 sites that were once part of the NGMP but are no longer actively monitored. Information on aquifer lithology, aquifer confinement and surrounding land use for each NGMP site is tabulated elsewhere (Rosen, 2001; Daughney and Reeves, 2005). Samples are collected from each NGMP site in March, June, September and December by regional council staff, following standard sampling guidelines (Rosen *et al.*, 1999). An unfiltered, unpreserved sample is analysed for alkalinity, conductivity and pH. Conductivity

and pH are also measured in the field where possible. A filtered (0.45 μm), unpreserved sample is analysed for Cl, Br, F, SO_4 , $\text{NO}_3\text{-N}$, $\text{NH}_4\text{-N}$ and $\text{PO}_4\text{-P}$. A filtered, acid-preserved (HNO_3) sample is analysed for Na, K, Ca, Mg, Fe, Mn and SiO_2 . Daughney and Reeves (2005) contains a detailed description of analytical methods that have been used throughout the history of the NGMP. Characteristics of the hydrochemical facies defined on the basis of median values of these parameters are presented in Tables 1 and 2.

Analytical results for each sample from each NGMP site were assessed for accuracy by calculation of the charge balance error (also termed the ion balance) following the method of Freeze and Cherry (1979). The acceptable limits for charge balance error for each sample were calculated by propagation of analytical uncertainties through the charge balance error equation, as described by Daughney and Reeves (2005). Using this method, the acceptable limits for charge balance error were roughly $\pm 5\%$ for most NGMP samples, but were as low as $\pm 1.5\%$ or as high as $\pm 6.5\%$ for samples with very high or very low concentrations of total dissolved solids, respectively. All samples with charge balance errors outside acceptable limits were excluded from the dataset prior to trend analysis.

Following data screening based on charge balance error, outliers were removed on a per-site and per-analyte basis. In this investigation, outliers were identified using a modified z -score approach (Rousseeuw and Leroy, 1987). This method compares the analytical result for each sample (x) to the median and median absolute deviation (MAD) for all results for the same parameter from the site in question:

$$z = \frac{(x - \text{median})}{MAD}$$

The median and median absolute deviation were determined for each parameter at each site using the log-probability regression method of Helsel and Cohn (1988), which is suitable for datasets containing censored values and multiple censoring thresholds (see also Daughney and Reeves, 2005; Lee and Helsel, 2005). Outliers were defined as having $z > 4$. Although a threshold of $z > 3$ is often used for outlier detection, an assessment of the NGMP data indicated that the criterion $z > 4$ was required to remove only those outlying values interpreted as resulting from errors in measurement or sampling methods.

Detection and estimation of trends

Methods for detecting and estimating trends have been reviewed by Loftis *et al.* (1991), Esterby (1996), Dixon and Chiswell (1996) and Hess *et al.* (2001). Trend detection involves analysis of time-series water quality data to determine if the values of particular parameters generally increase, generally decrease, or essentially remain the same over time. Trend detection is typically formulated as a two-sided hypothesis test that is performed at a defined confidence level, where the null hypothesis is that the result versus time relationship has a slope of zero. Where the test indicates a significant deviation from zero slope (i.e., rejection of the null hypothesis), a trend is said to exist for the particular parameter over the particular period of record. Trend estimation involves evaluation of the rate or amount of change over time. Trend magnitudes can be estimated using several different approaches, the more common based on Sen's slope estimator or linear regression (Helsel and Hirsch, 1992; Esterby, 1996).

In this investigation, we use the seasonal Mann-Kendall test ($\alpha = 0.05$) to detect trends in selected water quality parameters at each NGMP site. This test is non-parametric and therefore suitable for water quality data,

which are typically non-normally distributed (Helsel and Hirsch, 1992; Smith *et al.*, 1996). This test is also suitable for seasonally-variable data, as may be expected for shallow groundwaters. Of the various approaches to trend detection evaluated by Hess *et al.* (2001), the seasonal Mann-Kendall test was judged to be preferable because it maintains its stated α level and it maintains a high power with different trend functions. Absolute rates of change (units per year) are estimated using the seasonal Kendall Sen slope estimator and linear regression (Helsel and Hirsch, 1992; Smith *et al.*, 1996). Relative rates of change (% per year) are determined by dividing the absolute rate of change by the median value of the parameter at the site in question.

The methods described above were used to detect and estimate trends on a per-analyte basis for 153 NGMP sites. Trends were assessed for Br, Ca, Cl, F, Fe, HCO₃, K, Mg, Mn, Na, NH₄-N, NO₃-N, PO₄-P, SiO₂, SO₄, pH (field-measured), conductivity (lab-measured) and temperature (field-measured). Trend tests for pH were based on field measurements, because pH measured in the lab has a questionable relationship to *in situ* pH (Daughney and Reeves, 2003). For all parameters, censored results were replaced with one-half the highest detection limit for the purpose of trend testing, as recommended by Helsel and Hirsch (1992).

For each parameter at each NGMP site, trends were first assessed using the entire historical record of data, from the start of monitoring to December 2005. The length of record differed for each site, because regions joined the NGMP at different times and some sites have been removed from the NGMP over time for various reasons, but on average the period of record was seven years. To identify temporal patterns that are not constant over the entire record of data (i.e., not steadily increasing or steadily decreasing), trends were also assessed using

subsets of the historical record, involving data collected from January 1993 to December 1996, January 1997 to December 2000, or January 2001 to December 2005. Note that because of possible biases associated with autocorrelation, trend assessments valid for one particular time interval should not be extrapolated to later time periods (Loftis *et al.*, 1991).

Trend assessments were considered to have insufficient power, and were thus not performed, if the parameter of interest had not been measured at least eight times at the site in question within the time interval of interest. Although the power of trend tests can never actually be evaluated (Helsel and Hirsch, 1992), estimates of power can be obtained using Monte Carlo simulations (Yue *et al.*, 2002). These simulations show that the power of the Mann-Kendall test depends on the pre-selected significance level, the absolute magnitude of the trend, the number of observations, and the amount of variation within the interval of interest (Yue *et al.*, 2002). Because these relationships cannot be evaluated with the available data in this investigation, a minimum of eight samples was considered necessary for trend detection, following from the minimum sample sizes considered for trend detection in other groundwater systems (e.g., Frapporti *et al.*, 1994).

Hierarchical cluster analysis

Hierarchical cluster analysis was conducted using StatGraphics software. The cluster analysis was performed using *z*-scored rates of change of the following 15 water quality parameters: Br, Ca, Cl, F, Fe, HCO₃, K, Mg, Mn, Na, NH₄-N, NO₃-N, PO₄-P, SiO₂ and SO₄. Conductivity was excluded from the cluster analysis because, as a measure of total dissolved solids, it does not provide information not already encapsulated by the concentrations of major cations and anions.

pH was excluded from the cluster analysis because trends could not be assessed for a large number of sites for quite a few of the time intervals considered in this investigation, simply due to a lack of data (see below). Temperature was excluded from hierarchical cluster analysis because significant trends were detected at very few NGMP sites. The distributions of rates were non-normal for most analytes, and no transformation to produce near-normal distributions could be identified. Although this violates one of the central assumptions of hierarchical cluster analysis, it was decided that the cluster analysis would still provide a useful method for grouping the NGMP sites based on the rates of change of the selected water quality parameters.

For many analytes, rates could not be calculated because a large proportion of samples had concentrations below the analytical detection limit. For the hierarchical cluster analysis, rates that could not be calculated were replaced with zeros. This is not strictly accurate, because a significant trend could exist, even though all results remained below the analytical detection limit. However, consider the case where the concentration of a parameter is below a detection limit of 0.005 g m⁻³ for all samples collected within a four-year period (the length of the time intervals considered in this investigation). The maximum rate of change in concentration at this site is ±0.0013 g m⁻³ yr⁻¹. The positive value is based on the assumption that the concentration was zero for the first sample collected, was intermediate for subsequent samples, and was just below the detection limit for the last sample; the negative value assumes that concentrations decrease instead of increase with time. Thus for NGMP sites where concentrations have remained below the detection limit for at least four years, the median rate of change is probably close to zero.

In this investigation, several approaches for hierarchical cluster analysis were compared. Cluster analysis results were compared with 1) various combinations of linkage rules and similarity measures, 2) the use of absolute rates as opposed to relative rates, 3) the use of rates determined by the seasonal Kendall Sen slope estimator as opposed to linear regression, 4) the use of various treatments for non-detectable trends and for trends that could not be determined due to high censoring levels, and 5) the use of rates based on the entire historical data record (from the start of monitoring at each site until December 2005) as opposed to rates based on various four-year subsets of the data record.

The most appropriate method for hierarchical cluster analysis was selected based on the robustness and interpretability of the results. First, for each method, the robustness of hierarchical cluster analysis was assessed using an iterative method in which up to 20% of the sites or up to three analytes were randomly excluded. The methods of hierarchical cluster analysis that were least affected by exclusion of sites or analytes were identified as most robust. Second, the results of hierarchical cluster analysis were assessed for their interpretability—those methods that produced groups of sites with the most obvious relationships to hydrochemistry, site location, aquifer type, etc. were selected as most interpretable. This method of identifying the most appropriate method for hierarchical cluster analysis combines objective and subjective elements to identify the approach that is most suitable for the aims of this investigation.

Hierarchical cluster analysis places sites into groups based on their similarity or dissimilarity, but it does not provide information about what makes the groups different, or how significant differences between the groups actually are. To obtain this information, the significance of varia-

tion of each analyte between clusters was assessed with the Kruskal-Wallis test. Several graphical methods, such as bivariate scattergrams and box-and-whisker plots were used to elucidate the major differences in the rates of change in each analyte between the clusters identified by hierarchical cluster analysis. Relationships between cluster assignments and categorical variables such as region, aquifer lithology, aquifer confinement and surrounding land use were assessed using the chi-square test.

Results

Detection and estimation of trends

For most parameters, when the entire historical record of data is considered (to maximise statistical power), a significant increasing or decreasing trend is evident at roughly 25% of NGMP sites (Table 3). For most parameters, the proportions of sites showing increasing and decreasing trends are the same to within 10%. Exceptions include Cl, K, NO₃-N, PO₄-P and conductivity, for which the proportion of sites showing increasing trends exceeds the proportion of sites showing decreasing trends by more than 10%, and Na, which shows the opposite pattern. Similar observations were made by Frapporti *et al.* (1994) for shallow groundwaters in the Netherlands, where the increasing trends in NO₃-N and K were attributed to intensification of agricultural activity, and the decreasing trend in Na was ascribed to a decrease in evapotranspiration associated with declining water tables. For most parameters, trend assessments indicate no detectable change at approximately 50% of NGMP sites, although we acknowledge that, due to the low number of observations available at some sites, the power to detect trends is limited. Of the NGMP sites considered in this investigation, 16% had data records too short to permit a robust assessment of trends (i.e., fewer than eight samples collected).

Table 3 – Percentage of NGMP sites ($n = 153$) with significantly increasing (Inc) or decreasing (Dec) trends ($\alpha = 0.05$) for selected parameters, based on the entire historical record (period ending December 2005). %NDC represents the percentage of sites showing no detectable change over time; %ND represents the percentage of sites for which trend calculations could not be performed.

Parameter ¹	%Inc	%Dec	%NDC	%ND
Br	14	21	39	26
Ca	12	20	52	16
Cl	27	11	46	16
F	12	4	64	20
Fe	14	12	50	24
HCO ₃	17	18	49	16
K	21	5	58	16
Mg	16	14	53	16
Mn	3	20	41	35
Na	7	27	50	16
NH ₄ -N	4	5	66	25
NO ₃ -N	22	6	54	19
PO ₄ -P	16	1	44	39
SiO ₂	7	12	65	16
SO ₄	19	15	50	16
Conductivity	30	8	39	23
pH	5	4	55	37
Temperature	6	4	69	21

¹ pH and temperature are measured in the field; all other parameters are measured in the laboratory.

Trends could not be assessed for certain heavily censored parameters (e.g., PO₄-P, Mn, Fe, Br) at an additional 15-20% of the NGMP sites. Field pH measurements have been made only sporadically throughout the history of the NGMP, and so trends could not be assessed at 37% of the NGMP sites considered in this study.

Median rates of change for selected parameters are presented in Table 4, based on the seasonal Kendall Sen slope estimator, for the period from the start of monitoring at

each site until December 2005 (all NGMP sites are considered as a single group). Selected percentiles in absolute rates of change are listed in Table 5. Similar values for these percentiles are obtained for the entire historical data record, or when the analyses are limited to any other four-year subset of the historical record (results not tabulated). The seasonal Kendall Sen slope estimator and the linear regression method produced very similar estimates of rate of change, with median rates of change close to zero for most analytes. Compared to the relevant median values from Daughney and Reeves (2005), this equates to median relative rates of change of less than $\pm 3\%$ per year for all parameters considered in this investigation (Table 4). There is certainly some bias introduced into the calculated rates of change by having to replace censored values with one-half the highest detection limit during the trend assessments (Helsel and Hirsch, 1992). It is not possible to estimate the magnitude of this bias, but it may be significant for certain parameters at certain sites, where more than 5% of analytical results are reported as being below some detection limit (Helsel and Hirsch, 1992).

For most analytes, absolute rates of change are uncorrelated or only weakly correlated to median values (Table 6). This is not surprising. Consider two sites with very low rates of change in conductivity. One site might be a shallow, young groundwater with conductivity $\approx 100 \mu\text{S cm}^{-1}$ that remains constant over time due to the constancy of the hydrochemistry of its recharge source (e.g., a river). The other site might be an older, deep groundwater with a conductivity $\approx 700 \mu\text{S cm}^{-1}$ that remains constant over time because it has reached equilibrium with respect to the aquifer minerals. This example shows that lack of change in chemistry cannot be unequivocally related to 'security' (cf. Close *et al.*, 2000); the deep site might be relatively secure, but the shallow site

Table 4 – Median values, median absolute rates of change based on the seasonal Kendall Sen slope estimator, and median relative rates of change of selected water quality parameters, based on the entire historical record for each site (period ending December 2005).

Parameter ¹	Units	Median Value ²	Median Absolute Rate (units per year)	Median Relative Rate (% per year)
Br	g m ⁻³	0.06	0.000	0
Ca	g m ⁻³	15.9	0.064	0.4
Cl	g m ⁻³	14.0	0.000	0
F	g m ⁻³	0.07	0.000	0
Fe	g m ⁻³	0.03	0.000	0
HCO ₃	g m ⁻³	82.0	-0.185	-0.2
K	g m ⁻³	1.70	0.035	0.2
Mg	g m ⁻³	5.8	0.010	0.2
Mn	g m ⁻³	<0.01	0.000	ND
Na	g m ⁻³	15.4	-0.387	-2.5
NH ₄ -N	g m ⁻³	<0.01	0.000	ND
NO ₃ -N	g m ⁻³	0.77	0.000	0
PO ₄ -P	g m ⁻³	0.01	0.000	0
SiO ₂	g m ⁻³	23.0	0.297	1.3
SO ₄	g m ⁻³	5.5	-0.001	-0.02
Conductivity	µS cm ⁻¹	220.0	2.704	1.2
pH	pH units	6.89	-0.019	-0.3
Temperature	°C	14.7	-0.009	-0.1

¹ pH and temperature are measured in the field; all other parameters are measured in the laboratory.

² Median value of each parameter based on Daughney and Reeves (2005).

Table 5 – Percentiles in absolute seasonal Kendall Sen slope estimator rates of change in selected water quality parameters for all NGMP sites considered as a single group, based on the entire historical record for each site (period ending December 2005).

Parameter ¹	Units	Percentiles, Absolute Rates of Change (units per year)				
		5th	25th	50th	75th	95th
Br	g m ⁻³	-0.017	-0.003	0.000	0.007	0.016
Ca	g m ⁻³	-1.550	-0.119	0.064	0.255	1.010
Cl	g m ⁻³	-1.518	-0.116	0.000	0.207	1.701
F	g m ⁻³	-0.006	-0.002	0.000	0.003	0.011
Fe	g m ⁻³	-0.039	-0.004	0.000	0.000	0.056
HCO ₃	g m ⁻³	-4.759	-1.003	-0.185	0.257	2.315
K	g m ⁻³	-0.092	0.000	0.035	0.087	0.257
Mg	g m ⁻³	-0.245	-0.033	0.010	0.083	0.317
Mn	g m ⁻³	-0.011	0.000	0.000	0.000	0.011
Na	g m ⁻³	-2.779	-0.620	-0.387	-0.097	0.242
NH ₄ -N	g m ⁻³	-0.003	0.000	0.000	0.000	0.036
NO ₃ -N	g m ⁻³	-0.334	-0.012	0.000	0.016	0.296
PO ₄ -P	g m ⁻³	-0.005	0.000	0.000	0.002	0.008
SiO ₂	g m ⁻³	-0.242	0.006	0.297	0.620	1.291
SO ₄	g m ⁻³	-0.970	-0.075	-0.001	0.058	0.904
Conductivity	µS cm ⁻¹	-9.289	-4.681	2.704	7.525	21.673
pH	pH units	-0.742	-0.073	-0.019	0.035	0.642
Temperature	°C	-0.705	-0.106	-0.009	0.050	0.428

¹ pH and temperature are measured in the field; all other parameters are measured in the laboratory.

Table 6 – Regression models relating absolute seasonal Kendall Sen slope estimator rate of change to median value, considering all NGMP sites as a single group and based on the entire historical record for each site (period ending December 2005).

Parameter ¹	Slope ²	Intercept ²	r ³
Br	-0.055	0	-0.81
Ca	-0.018	0.170	-0.57
Cl	0	0	NA
F	0	0	NA
Fe	0.082	0	0.48
HCO ₃	0	0	NA
K	0.026	0	0.63
Mg	0	0	NA
Mn	-0.022	0	-0.58
Na	-0.017	0	-0.44
NH ₄ -N	0.029	0	0.93
NO ₃ -N	-0.017	0.122	-0.38
PO ₄ -P	0.051	0	0.46
SiO ₂	-0.013	0	-0.44
SO ₄	0.053	-0.365	0.51
Conductivity	0	0	NA
pH	0	0	NA
Temperature	0	0	NA

¹ pH and temperature are measured in the field; all other parameters are measured in the laboratory.

² Slope and intercept of the regression model; zeros represent cases where slope or intercept does not differ significantly from zero ($p > 0.05$).

³ Pearson correlation coefficient

might be quite vulnerable to chemical contamination.

The Kruskal-Wallis test (Helsel and Hirsch, 1992) was employed to test for significant differences in the absolute rates based on the following categorical variables: regional council, aquifer lithology, aquifer confinement, use of surrounding land, and hydrochemical facies (see Daughney and Reeves, 2005). Tests were performed using absolute rates calculated using the entire historical record of data for each NGMP site (i.e., from the start of monitoring at each

site until December 2005), and various four-year subsets of the data record as described above. Test results indicate that there are no parameters for which absolute rates of change vary significantly as a function of any of these categorical variables ($p > 0.05$) when all NGMP sites are considered as a single group (test results not tabulated).

Hierarchical cluster analysis: method selection

To identify the most appropriate method for hierarchical cluster analysis, we compared various combinations of the seven linkage rules and three similarity measures supported by the StatGraphics software. The square of the Euclidean distance (E^2) provided the best measure of similarity between samples and clusters. This similarity measure places progressively greater weight on samples that are further apart, and so emphasises differences that tend to be dampened by other similarity measures (e.g., City Block distance). Two linkage rules were found to be most useful. The nearest-neighbour linkage rule was used to identify sites that bore very little resemblance to any others (residuals). Ward's linkage rule was used to define clusters for sites not identified as residuals. Ward's method is based on an analysis of variance, and produces smaller distinct clusters than other linkage rules, such that each observation in a cluster is more similar to other observations in the same cluster than to any observation from any other cluster. The combination of the square of the Euclidean distance with the nearest-neighbour or Ward's linkage rule has been shown to be most effective for classification of groundwater monitoring sites based on the median values of water quality parameters (Güler *et al.*, 2002; Daughney and Reeves, 2005).

Comparable results were obtained from hierarchical cluster analysis using absolute rates instead of relative rates. However, interpretation of results based on relative rates

was more complex, because the clustering is dependent on twice as many input variables (i.e., rate of change and median value for each parameter). For this reason, in this study we present results obtained from hierarchical cluster analysis of absolute rather than relative rates.

Comparable results were obtained when hierarchical cluster analysis was performed using rates estimated by the seasonal Kendall Sen slope estimator as opposed to linear regression. This is because the seasonal Kendall Sen slope estimator and the linear regression method produced very similar estimates of rate of change for most parameters at most sites. Hierarchical cluster analysis based on the seasonal Kendall Sen slope estimator resulted in slightly lower separation measures between sites within a single cluster. This is because the slope estimator, as an indicator of median rate of change, can be equal to zero for several parameters at several sites within a single cluster. Rates estimated by linear regression, however, are typically not equal to zero and thus differ slightly between sites within a single cluster. The slightly lower separation measures did not affect interpretation of the results, and so hierarchical cluster analysis was performed using rates based on the seasonal Kendall Sen slope estimator in order to avoid possible biases associated with rate estimation by the linear regression method (Helsel and Hirsch, 1992; Esterby, 1996; Hess *et al.*, 2001).

We also tested the effect of performing hierarchical cluster analysis using two different treatments for non-significant trends. In the first case, hierarchical cluster analysis was conducted using rates determined using the seasonal Kendall Sen slope estimator, regardless of whether or not a significant trend had been identified by the Mann-Kendall test. In the second case, if the trend in any parameter was not significant at a particular site, the rate based on the slope estimator was replaced with a zero. These two

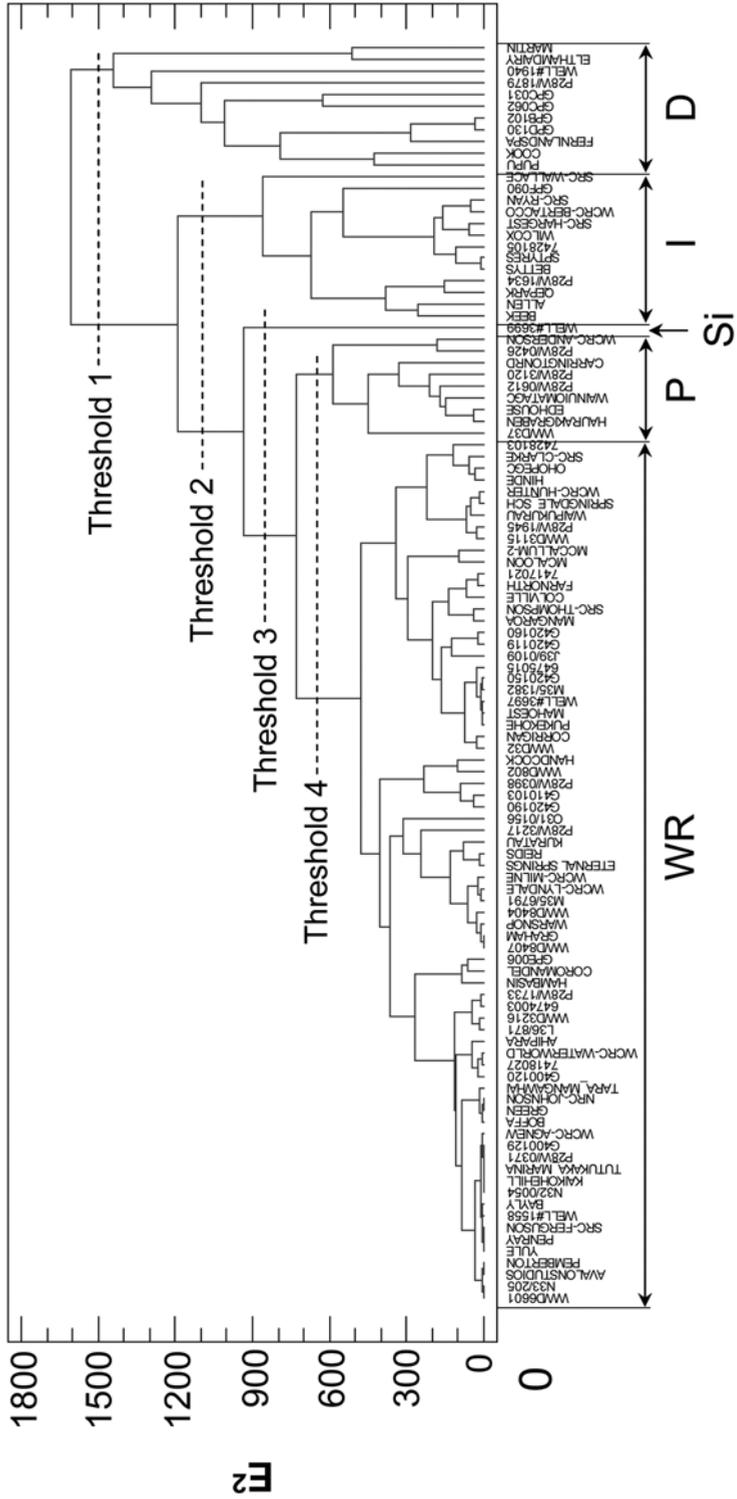
approaches produced similar results, except that the former resulted in greater separation between sites, simply because the rates were different (i.e., non-zero) for most sites, even within a single cluster. Thus, to allow for maximum resolution, all results presented in this communication pertain to hierarchical cluster analysis conducted using rates for both significant and non-significant trends.

Finally, we evaluated the effect of performing hierarchical cluster analysis using rates based on the entire historical record of data for each site (period ending December 2005), compared to rates based on various four-year subsets of the data record. In general, comparable results were obtained using these two approaches. However, several sites exhibited trends that were not steadily increasing or steadily decreasing over the longer interval. We therefore concluded that hierarchical cluster analysis conducted with rates calculated from the four-year subsets of the data record would provide more insight into the geochemical processes involved.

Hierarchical cluster analysis: characteristics of clusters

Three NGMP sites could be classified as residuals as a result of hierarchical cluster analysis conducted with the nearest neighbour linkage rule, based on seasonal Kendall Sen slope estimator rates calculated using data collected from January 2001 to December 2005. One site identified as a residual (Tutukaka_Mar_2, Northland Regional Council) differed from all other sites in showing a very rapid decreases in Na ($-33 \text{ g m}^{-3} \text{ yr}^{-1}$), Cl ($-21 \text{ g m}^{-3} \text{ yr}^{-1}$) and SO_4 ($-68 \text{ g m}^{-3} \text{ yr}^{-1}$), possibly associated with a decreasing marine influence over time. The second site identified as a residual (WWD3314, Tasman District Council) was characterised by rapidly increasing HCO_3 ($4.5 \text{ g m}^{-3} \text{ yr}^{-1}$), Fe ($0.2 \text{ g m}^{-3} \text{ yr}^{-1}$) and Mn ($0.01 \text{ g m}^{-3} \text{ yr}^{-1}$), accompanied by decreasing $\text{NO}_3\text{-N}$ ($-0.06 \text{ g m}^{-3} \text{ yr}^{-1}$). This pattern of

Figure 1 – Dendrogram for non-residual NGMP sites, based on seasonal Kendall Sen slope estimator rates of change of 15 chemical parameters (January 2001 to December 2005) and Ward's linkage rule and the square of the Euclidean distance (E^2) as the separation measure.



hydrochemical change is probably related to the development of anoxic conditions, possibly related to changes in land use around the site (see Rosen, 1999). The third site identified as a residual (Reesby (now called 362791), Manawatu-Wanganui Regional Council) was differentiated from all other sites by increasing HCO_3 ($1.6 \text{ g m}^{-3} \text{ yr}^{-1}$), accompanied by rapidly decreasing Br ($-0.3 \text{ g m}^{-3} \text{ yr}^{-1}$), Na ($-1.0 \text{ g m}^{-3} \text{ yr}^{-1}$) and SiO_2 ($-1.1 \text{ g m}^{-3} \text{ yr}^{-1}$). The cause of these changes in hydrochemistry is not clear, but the decrease in Br may be related to a reduction in the use of Br-based fumigants in the area around the site. Because of the unusual temporal patterns in hydrochemistry at these three sites, they were excluded from further hierarchical cluster analysis in order to eliminate possible biasing effects.

Hierarchical cluster analysis conducted with Ward's linkage rule, without the three sites identified as residuals, produces the dendrogram displayed in Figure 1. As above, hierarchical cluster analysis was performed using seasonal Kendall Sen slope estimator rates based on data collected from January 2001 to December 2005. This dendrogram indicates that the non-residual NGMP sites having sufficient data for the period of interest ($n = 108$) can be partitioned into up to five groups, based on the progressive lowering of a threshold value for the separation measure. In most cases, each separation threshold differentiates about ten sites from the remaining majority. We designate these groups as Clusters D, I, Si, P and WR, with characteristic rates of change summarised in Table 7. These names have been selected for specific reasons that are summarised in Table 8 and described in detail below. Note that the trend-based clusters described in this paper are distinct from the hydrochemical facies defined by Daughney and Reeves (2005) (Tables 1 and 2). Locations of NGMP sites falling into particular trend-based clusters are displayed in Figure 2.

At the highest separation threshold ($E^2 = 1500$), we define Cluster D, a group of 11 sites that is differentiated from the remaining 99 sites. The Kruskal-Wallis test indicates that the sites in Cluster D are distinguished from the remaining sites by much more rapid decreases in Na, Ca, HCO_3 and Cl over time (rates of change of other parameters do not differ significantly between the two groups) (Table 7). Na, Ca, HCO_3 and Cl typically represent a significant proportion of the total ionic charge in most groundwaters, and a simultaneous decrease in all four analytes is indicative of a reduction in the total concentration of dissolved solids. Assignment of sites to Cluster D is not related to aquifer lithology or confinement, or use of the surrounding land, but site location is important, with seven of the sites in Cluster D in either the Gisborne or Hawke's Bay region (Figure 2). Sites in Cluster D have a median depth of 95 m below ground surface, compared to the median depth of 27 m for all other sites. The sites in Cluster D have relatively high concentrations of most parameters and conductivities in the range $535\text{-}1700 \mu\text{S cm}^{-1}$, and are thus categorised as reduced, evolved groundwaters (hydrochemical facies 2A and 2B) by Daughney and Reeves (2005). We tentatively conclude that sites in Cluster D display a pattern of *dilution* over time of generally deep, geochemically evolved groundwaters. This may be the result of variable hydrologic conditions, possibly associated with human influence. For example, the groundwater at these sites may be increasingly influenced by dilute river recharge due to a changing pumping regime, with a concomitant reduction in the signature of more evolved, solute-rich groundwaters.

At the second separation threshold ($E^2 = 1100$), we define Cluster I, a group of 13 sites. The Kruskal-Wallis test indicates that sites in Cluster I display significantly more positive rates of change of Ca, Cl, K, Mg, Na,

Table 7 – Selected percentiles (%) in absolute seasonal Kendall Sen slope estimator rates of change ($\text{g m}^{-3} \text{yr}^{-1}$) in clusters defined by hierarchical cluster analysis.

Cluster	%	Br	Ca	Cl	F	Fe	HCO ₃	K	Mg	Mn	Na	NH ₄ -N	NO ₃ -N	PO ₄ -P	SiO ₂	SO ₄
	5	-0.035	-6.643	-7.658	-0.003	-0.464	-8.418	-0.091	-0.741	-0.012	-8.553	-0.019	-0.307	-0.007	-0.528	-2.696
	25	-0.015	-2.923	-3.582	-0.001	-0.020	-3.861	0.002	-0.160	-0.003	-5.638	0.001	0.000	0.000	-0.141	-1.570
D	50	0.007	-0.615*	-0.838*	0.001	-0.001	-1.025*	0.141	0.000	0.000	-1.880*	0.016	0.000	0.002	0.437	0.000
	75	0.017	-0.082	-0.111	0.012	0.020	-0.202	0.337	0.113	0.002	-0.269	0.083	0.002	0.006	0.936	0.010
	95	0.023	0.965	0.825	0.022	0.060	1.241	0.562	0.365	0.017	1.506	0.179	0.004	0.037	1.490	0.331
	5	-0.010	-0.012	-0.779	-0.005	-0.047	-4.956	0.023	0.033	-0.008	-0.615	-0.003	-0.004	-0.006	-0.049	-0.115
	25	0.000	0.238	0.053	-0.001	-0.010	-2.062	0.068	0.129	0.000	-0.426	0.000	0.006	0.000	0.250	-0.052
I	50	0.002	0.488*	1.005*	0.002	0.000	-0.540	0.133*	0.238*	0.000	-0.131	0.000	0.274*	0.000	0.311	0.396*
	75	0.010	0.885	2.587	0.003	0.000	0.000	0.168	0.314	0.000	0.093	0.000	0.376	0.002	0.613	1.611
	95	0.015	1.292	4.767	0.009	0.098	3.772	0.271	0.425	0.043	0.338	0.010	0.594	0.002	1.807	3.998
Si	N/A	0.002	0.246	0.017	-0.001	-0.022	2.243	-0.097	-0.062	0.031	0.000	0.037	-0.014	-0.003	3.788*	0.009
	5	-0.004	-0.704	-0.171	-0.032	-0.004	-5.583	-0.390	-0.646	0.000	-1.141	-0.002	-0.728	0.000	0.250	-0.941
	25	-0.002	-0.125	-0.126	-0.015	-0.002	-1.136	-0.149	-0.236	0.000	-0.468	0.000	-0.611	0.000	0.413	-0.331
P	50	0.000	-0.038	-0.025	-0.004	0.000	0.000	-0.057*	-0.141*	0.000	-0.092	0.000	-0.372*	0.000	0.466	-0.059
	75	0.000	0.023	0.151	0.002	0.000	0.181	-0.003	0.000	0.000	-0.002	0.000	-0.013	0.002	0.504	0.000
	95	0.008	0.425	0.722	0.009	0.002	3.139	0.062	0.121	0.000	0.219	0.000	-0.001	0.003	0.981	0.216
	5	-0.014	-0.638	-0.642	-0.006	-0.039	-3.045	-0.024	-0.166	-0.010	-1.330	-0.001	-0.119	-0.003	-0.169	-0.818
	25	-0.004	-0.039	-0.061	-0.001	-0.001	-0.771	0.001	-0.029	0.000	-0.590	0.000	-0.011	0.000	0.000	-0.074
WR	50	0.000	0.058	0.000	0.000	0.000	-0.067	0.028	0.010	0.000	-0.387	0.000	0.000	0.000	0.221	-0.002
	75	0.005	0.201	0.108	0.003	0.000	0.297	0.070	0.059	0.000	-0.136	0.000	0.016	0.002	0.557	0.050
	95	0.014	0.665	0.690	0.007	0.035	1.511	0.150	0.193	0.004	0.000	0.015	0.143	0.007	1.011	0.389

* Denotes parameter that differ significantly between categories at the relevant threshold (Kruskal-Wallis test, $p < 0.05$)

Table 8 – General characteristics of trend-based clusters in the NGMP defined by hierarchical cluster analysis.

Cluster	<i>n</i>	Temporal pattern	Possible causes	Comments
D (dilution)	11	Rapid decrease in Na, Ca, HCO ₃ and/or Cl over time	Change in pumping regime or hydrogeologic conditions	<ul style="list-style-type: none"> Typically hydrochemical facies 2 Median depth 95 m 7 out of 11 found in either Gisborne or Hawke's Bay regions No significant relationship to lithology, confinement or surrounding land use
I (impact)	13	Increases in Ca, Cl, K, Mg, Na, NO ₃ -N and/or SO ₄ over time	Increasing proportion of recharge from rainfall relative to rivers over time, increasing human/agricultural impact in recharge area	<ul style="list-style-type: none"> Typically hydrochemical facies 1 Median depth less than 10 m Most in unconfined aquifers No significant relationship to regional council, lithology or surrounding land use
Si	1	Rapid increase in SiO ₂ without accompanying changes in other analytes at a similar rate	?	<ul style="list-style-type: none"> With only one site, the significance of this cluster is questionable
P (pristine)	9	Decreases in K, Mg and/or NO ₃ -N over time, often with accompanying decreases in Ca, Na, Cl and/or SO ₄	Increasing proportion of recharge from rivers relative to rainfall over time, decreasing human/agricultural impact in recharge area	<ul style="list-style-type: none"> Typically hydrochemical facies 1 No significant relationship to depth No significant relationship to regional council, lithology, confinement or surrounding land use
WR (water-rock)	74	No or only slow changes in most analytes over time	Natural water-rock interaction	<ul style="list-style-type: none"> No significant relationship to hydrochemical facies No significant relationship to depth No significant relationship to regional council, lithology, confinement or surrounding land use

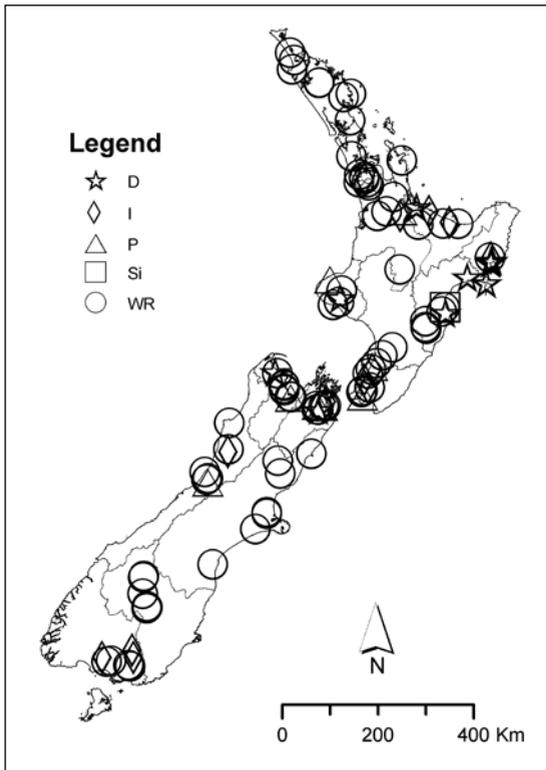


Figure 2 – Locations of NGMP sites in trend-based clusters defined by hierarchical cluster analysis. Regional authority boundaries are shown by solid lines.

$\text{NO}_3\text{-N}$ and SO_4 compared to the remaining 86 sites (Table 7). All of these substances can be accumulated during passage of rainfall recharge through the soil zone. Notably, Cl , $\text{NO}_3\text{-N}$ and SO_4 are increasing over time at sites in Cluster I, but in general show little or no detectable change over time at most of the remaining 86 sites. Accumulation of Cl , $\text{NO}_3\text{-N}$ and SO_4 in groundwater is consistent with increasing human or agricultural activities. We thus tentatively conclude that the temporal pattern that characterises Cluster I might arise from increasing human or agricultural impact over time, or an increased proportion of rainfall recharge relative to river recharge over time, or a combination of the two. We note that region,

aquifer lithology and surrounding land use do not appear to be related to the cluster assignment at this separation threshold. However, the majority of sites in Cluster I are in unconfined aquifers, and half are less than 10 m deep. All but three of the sites in Cluster I are in hydrochemical facies 1, meaning they are surface-dominated (Daughney and Reeves, 2005). Of these sites, all but three are in hydrochemical facies 1A, indicating probable human impact. The implication of the trend-based clustering is that these sites are becoming more affected with time. There are three sites in Cluster I that fall into hydrochemical facies 1B: at present they show little evidence of human impact and low median concentrations of $\text{NO}_3\text{-N}$ and Cl . The trend-based clustering, however, suggests that these sites may not remain so pristine in the future.

At the third separation threshold ($E^2 = 900$), we define Cluster Si, which contains only one site (Well#3699, Hawke's Bay Regional Council). The Kruskal-Wallis test indicates that the site in Cluster Si is differentiated from the remaining 85 sites mainly by a significant rise in SiO_2 (Table 7), which has increased steadily from $1\text{-}2\text{ g m}^{-3}$ in 1999 to roughly 27 g m^{-3} in 2004-2005. This site also exhibits increases in HCO_3 and Mn , but overall, hydrochemical trends in parameters other than SiO_2 are not sufficiently unusual for this site to be categorised as a residual. The cause of the temporal pattern at Well#3699 is unclear. This site is in a confined aquifer comprising fluvial post-glacial gravel. The concentrations of SiO_2 observed at this site in 1999 are much lower than would be expected for any natural water, although the current concentrations are typical of groundwater. Other analytes do not display matching trends that might allow the cause of the trends in SiO_2 , HCO_3 and Mn to be elucidated,

and because Cluster Si contains only one site, its relevance at the national scale is questionable.

At the fourth separation threshold ($E^2 = 600$), we define Cluster P, containing nine sites that are distinguished from the remaining 74 sites. The Kruskal-Wallis test indicates that sites in Cluster P display significantly more negative rates of change of K, Mg and $\text{NO}_3\text{-N}$ compared to the remaining 74 sites (Table 7). Most of the sites in Cluster P also display decreases in Ca, Na, Cl and/or SO_4 . As with Cluster D, the simultaneous decrease in the concentrations of several major ions is indicative of a reduction in the total concentration of dissolved solids. However, compared to Cluster D, absolute rates of decrease in major ion concentration are lower (i.e., the changes occur more slowly) at sites in Cluster P. We note that most sites in Cluster P fall into hydrochemical facies 1A or 1B and thus have lower solute concentrations than the sites in Cluster D, which fall into hydrochemical facies 2A or 2B (see above). In addition, we observe that Cluster P is characterised by much more rapid decreases in $\text{NO}_3\text{-N}$ relative to Cl compared to Cluster D. We therefore tentatively conclude that Cluster P represents groundwaters that are becoming more *pristine* over time. This temporal pattern is essentially the opposite of Cluster I. Cluster P sites appear to show less human or agricultural impact over time, or an increased proportion of river recharge relative to rainfall recharge over time, or a combination of the two. Cluster P is not differentiated from other trend-based clusters on the basis of aquifer lithology, aquifer confinement, surrounding land use or region.

Finally, we define Cluster WR, which contains the 74 NGMP sites that are not assigned to any of the other trend-based clusters at separation threshold $E^2 = 600$. The majority of sites in Cluster WR show

no detectable changes, or only slow changes in most parameters over time (Table 7) that we tentatively conclude might arise due to natural *water-rock interaction*.

Baseline rates of change

In this study, the range of rates of change defining the baseline for each parameter were determined using the 5th, 25th, 75th and 95th percentiles. A similar approach has been used in previous investigations to define baselines for the concentrations (as opposed to rates of change) of various water quality parameters (Barnes and Langmuir, 1978; Newcomb and Rimstidt, 2002; Lee and Helsel, 2005; Daughney and Reeves, 2005). Conservatively, the baseline can be defined as the range of rates between the 5th and 95th percentile of the relevant distribution, with an 'anomaly' defined as a rate of change above the 95th percentile or below the 5th percentile. The same approach can be applied on the 25th and 75th percentiles to provide a narrower definition of baseline rate of change. Percentiles in the rates of change determined when all NGMP sites are considered as a single group are given in Table 5; following the method of Daughney and Reeves (2005), percentiles are also calculated separately for each trend-based cluster defined by hierarchical cluster analysis (Table 7).

There are two caveats to the baseline definitions used in this investigation. First, if the goal is to define the 5th and 95th percentiles of a distribution of *natural* rates of change, then the distribution must not contain values that are representative of *abnormal* rates of change that might be caused by human impact. To illustrate by analogy, Newcomb and Rimstidt (2002) presented distributional models based on all of the data in the United States Environmental Protection Agency database. This database contains analytical results for groundwaters collected across the United States, including

groundwaters from contaminated sites, and so the 5th and 95th percentiles defined from the dataset should not be considered to be indicative of the range of concentrations in normal (unaffected) groundwaters (Lee and Helsel, 2005). Daughney and Reeves (2005) defined baseline concentrations of selected analytes in New Zealand groundwaters through the use of hierarchical cluster analysis, which allowed groundwaters showing probable evidence of human impact to be identified and excluded from the baseline models. A second caveat concerns the number of sites from which data have been collected. In this investigation, baseline rates of change are defined based on data from NGMP sites. The NGMP constitutes a small portion of the groundwater monitoring actually conducted in New Zealand, and it is not yet clear whether the NGMP sites represent the full range of conditions and hydrochemistries found throughout the country. If baseline models are developed in the future using additional monitoring sites, the threshold values presented in this paper may change.

As an example of the approach outlined above, we define indicative baseline rates of change for $\text{NO}_3\text{-N}$ in New Zealand's groundwaters. If all of the NGMP sites are considered as a single group, then it might appear that normal rates of change of $\text{NO}_3\text{-N}$ in groundwater could range from -0.3 to $+0.3 \text{ g m}^{-3} \text{ yr}^{-1}$, based on the 5th and 95th percentiles listed in Table 5. However, this range of rates is biased by inclusion of sites in Clusters D, I, Si and P, at which relatively rapid hydrochemical changes may be occurring as a result of human or agricultural impact. We thus suggest that a more appropriate definition of baseline is based on the range of rates observed for Cluster WR. Thus, the baseline rate of change of $\text{NO}_3\text{-N}$ in New Zealand groundwaters that are not affected by human or agricultural activity should be less than $\pm 0.1 \text{ g m}^{-3} \text{ yr}^{-1}$, based on the 5th and 95th percentiles in Table 7.

Discussion

The interpretation of temporal trends in groundwater quality is not straightforward. The general assumption is that changes in land use should affect groundwater quality and give rise to easily detectable temporal trends. Working on this premise, previous investigations have evaluated temporal trends in indicator compounds such as $\text{NO}_3\text{-N}$ that would be expected to increase in concentration in groundwater as a result of particular land-use practices (e.g., Close, 1987; Close *et al.*, 1995; Reijnders *et al.*, 1998; Broers and van der Grift, 2004). However, these investigations revealed fewer significant temporal trends in groundwater quality than anticipated. There are several reasons why temporal trends in groundwater can be difficult to detect and interpret, including the long travel times of groundwater to the monitoring sites, dissolution or precipitation of salts associated with changes in water level, dilution or concentration of substances due to changes in recharge volume or chemistry, changes in flow direction, and the non-conservative behaviour of the substance(s) of interest (Close *et al.*, 1995; Broers and van der Grift, 2004; Broers *et al.*, 2005; Foster, 2005).

Despite the difficulties associated with the detection of temporal trends in groundwater quality, this study has revealed significant trends in hydrochemistry at roughly 25% of the monitoring sites in the NGMP. The NGMP sites are selected to provide an 'early warning' of changing groundwater quality and are therefore located proximal to but not immediately in the aquifer recharge area (Rosen, 1999). In addition, the majority of the NGMP wells are shallow, with 25% and 50% of the sites having depths of less than 10 m and 25 m, respectively. Several previous investigations have shown that trends in groundwater quality are most easily detected in shallow groundwaters (e.g., on the basis

of concentration-depth data), especially in aquifer recharge areas (e.g., Dillon, 1989; Broers and van der Grift, 2004; Broers *et al.*, 2005; Foster, 2005). We observe that half of the sites assigned to Cluster I have depths of less than 10 m, but partitioning of sites into clusters at other separation thresholds does not reveal a significant relationship to well depth. This may be related to differences in groundwater age, which we aim to elucidate with a water dating survey of the NGMP sites that is underway as of January 2006. A future investigation will also address temporal trends in water level, and their relationship, if any to changes in hydrochemistry.

Very few national-scale assessments of temporal trends in groundwater quality are available for comparison to results reported here (see Loftis, 1996). Rosen (1999) evaluated temporal patterns in the NGMP data, but did not report rates of change or assess trends statistically. Frapporti *et al.* (1994) and Broers and van der Grift (2004) assessed rates of change in groundwater quality in The Netherlands. Broers and van der Grift (2004) detected significant trends in K, NO₃-N and the sum of cations (comparable to conductivity) at 42%, 8% and 35% of monitoring sites ($n = 13$ shallow + 13 deep sites), respectively, in a region of intensive livestock farming. The median absolute rates of change in New Zealand's groundwater quality (Table 5) are similar to the median rates reported by Broers and van der Grift (2004) for K (1.9 and 0.49 g m⁻³ yr⁻¹ in shallow and deep wells, respectively) and NO₃-N (0 g m⁻³ yr⁻¹ in shallow and deep wells). Comparisons to trends in groundwater quality in other countries must be made with caution, due to possible biases arising from differences in monitoring programme design, monitoring objectives, sampling and analytical methods, data interpretation techniques and so on (Dixon and Chiswell, 1996), not to mention differences in current and historical land-use practices. Still, at a

broad level at least, temporal trends in New Zealand groundwater quality appear to be similar to trends observed in other countries.

Although trends in river water and groundwater quality are not necessarily comparable, national-scale assessments of trends in New Zealand's river water quality are available for comparison to the results presented here. Smith *et al.* (1996) evaluated long-term trends in the water quality of New Zealand's rivers for the period 1989-1993 ($n = 77$ sites). Compared to the NGMP sites (Table 3), the river water monitoring sites showed similar proportions of detectable trends in conductivity (increasing trends at 39% of sites, decreasing trends at 9% of sites) and NH₄-N (increasing trends at 4% of sites, decreasing trends at 17% of sites), but very different proportions of detectable trends in NO₃-N (increasing trends at 5% of sites, decreasing trends at 38% of sites). Smith *et al.* (1996) reported national relative flow-adjusted rates of change in NO_x (4.4% yr⁻¹) and conductivity (0.7% yr⁻¹) in New Zealand's rivers that are similar to the national median relative rates of change in groundwaters presented in Table 4. Scarsbrook *et al.* (2003) described trends in New Zealand's river water quality for the periods 1989-1993, 1994-1998 and 1989-1998, and obtained results generally comparable to the earlier survey of Smith *et al.* (1996), although the results could also be interpreted in the context of climate variability. Based on a more recent data set (1996-2002), Larned *et al.* (2004) reported lower relative median flow-adjusted rates of change in NO_x (-0.04% yr⁻¹) and conductivity (0.07% yr⁻¹) in New Zealand's rivers. Overall, patterns of detectable trends and relative rates of change in certain analytes appear to be generally similar in New Zealand's rivers and groundwaters, but we stress that additional research is required to draw meaningful conclusions from any such comparison.

Summary and conclusions

Hierarchical cluster analysis was found to be a useful tool for interpretation of temporal trends in the NGMP data. Hierarchical cluster analysis does not require *a priori* assumptions about how many clusters there should be, or of the pattern of hydrochemical change each cluster should display. Although several different approaches can be employed in hierarchical cluster analysis, most methods produced comparable results, indicating that the methods are suitably robust for application to trends in water quality. Hierarchical cluster analysis allows for comparison of trends in groundwater quality between different regions of New Zealand. This proved very useful for the NGMP data set, which typically has just one monitoring site in a given aquifer and covers only about half of the major aquifers in New Zealand. In many cases, temporal trends in groundwater quality at a site in one region showed little resemblance to temporal patterns at other sites in the same region but were similar to patterns at sites in other regions. Hierarchical cluster analysis thus provided useful information about temporal trends in New Zealand's groundwaters by allowing holistic comparison across regions.

We tentatively conclude that the five trend-based clusters recognised by hierarchical cluster analysis represent specific patterns of trends in groundwater quality that might be associated with specific causes (Table 8). Variations in the rates of change in hydrochemistry appear to differentiate patterns associated with natural water-rock interaction from patterns associated with human influence. We recognise several different patterns of hydrochemical change associated with human influence, possibly arising from changes in pumping regime and/or changes in land use in the recharge zone. These trend-based clusters are based only on data from the NGMP, which

constitutes a relatively small proportion of the groundwater monitoring conducted in New Zealand, and the data records are short at several sites, which limits the statistical power to detect trends. It is therefore recommended that future studies should be conducted using longer time series records and additional data from monitoring sites outside the NGMP. It is also acknowledged that the drivers of change in water quality cannot be positively identified with the data presented in this investigation, and therefore it is recommended that age interpretations, water level measurements, and possibly climate data should be compared to the trend-based clusters defined here. Until such studies can be conducted, any non-NGMP monitoring site can be assigned to one of the trend-based categories defined in this investigation. This will provide a simple means of assessing temporal trends in water quality and assist with the development of appropriate groundwater resource management.

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