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Geospatial Modelling of Groundwater Quality in Semi-Arid Environments of South Africa

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Abstract Groundwater as a scarce freshwater resource requires extensive quality assessment, control and protection through innovative methods and efficient strategies in light of growing human population, pollution, and over–extraction. Groundwater is critical in arid and semi–arid regions of the world such as the Beaufort West area in the Karoo region of South Africa. Thus, this study investigated the key processes affecting groundwater quality using factor analysis and geospatial models to determine the spatial variability of groundwater quality. To achieve this objective, groundwater samples collected from 49 boreholes located in and around the town of Beaufort West and analysed for electrical conductivity (EC), pH, total dissolved solids (TDS), calcium (Ca^{2+}), magnesium (Mg^{2+}), sodium (Na^{+}), potassium (K^{+}), bicarbonates (HCO_3^{-}), chlorides (Cl^{-}), nitrates (NO_3^{-}) and sulphates (SO_4^{2-}) using recommended standard methods. Factor analysis produced three factors explaining 81.4% of groundwater quality variation. Factor 1 (hardness) was characterised by high concentrations of Cl^{-}, SO_4^{2-}, Ca^{2+}, Mg^{2+} and Na^{+}; factor 2 (alkalinity) with HCO_3^{-} and K^{+}, and factor 3 (anthropogenic) was characterised by high NO_3^{-} concentrations. Derived groundwater quality thematic maps using selected hydrochemical variables and factor scores showed the delineation of areas with hardness, alkalinity and anthropogenic influence on groundwater quality. These findings underscore the relevance of factor analysis and geospatial models in assessing groundwater quality at a catchment scale.

Keywords Arid Areas · Factor Analysis · Spatial Modelling · Water Quality · Water Resources Management

1 Introduction

Groundwater remains an important resource to urban and rural areas of the arid and semi–arid regions of the world, where surface water is scarce (Foster et al., 2012; Hoogesteger & Wester, 2015). Previous studies (e.g., Aizebeokhai, 2011; Taylor et al., 2009; Ziervogel et al., 2010) highlighted that increased groundwater utilisation is critical and can help to develop resilience to climate change, droughts and water scarcity for rural communities and countries, however, there is limited knowledge of groundwater quality and distribution patterns. Thus, groundwater resources are, therefore, increasingly relevant for drought adaptation in the arid and semi–arid regions of the world through

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the provision of a buffer to erratic and unreliable surface water availability during the dry season (i.e., or drought periods). These areas rely heavily on groundwater for domestic, irrigation and industrial activities, and understanding groundwater characteristics, quality and possible threats in such areas is of utmost importance in the management of such a scarce or unknown resource (Chen et al., 2018; Ebrahim et al., 2019; Hiscock & Bense, 2021).

Across the arid and semi–arid regions, most rural and urban communities rely on groundwater extracted from shallow wells since surface water is only available for a short period. However, literature shows that groundwater resources are directly or indirectly under strain from three major global social problems: human population, environment, and resources (Chen et al., 2018). Groundwater quality in arid and semi–arid areas is vulnerable to anthropogenic activities and high exposure to contaminants (Dalu et al., 2011; Masocha et al., 2019). Monitoring and management of groundwater quality and quantity in arid and semi–arid areas is fundamental in preserving this resource. Therefore, extensive research on groundwater quality and quantity is necessary.

Groundwater, a vital resource for drinking water, irrigation, and industrial use, faces a growing threat mostly from metal pollution (Alfaifi et al., 2021). This contamination arises from various human activities and natural processes, posing significant risks to human health and ecosystems. Metals, unlike many pollutants, are not readily biodegradable and can accumulate in the environment over time. When these metals infiltrate the ground, they can leach into groundwater resources, compromising their quality (Rajkumar et al., 2020). This introduction explores the concerning relationship between groundwater pollution and metal contamination, highlighting the sources of metal pollution and its detrimental effects. Groundwater chemistry is largely characterised by the mineral composition of the rocks it flows through and is normally explained as a water–rock interaction (Kurwadkar et al., 2020). While some metals naturally occur in rocks and soils, human actions significantly accelerate their release into groundwater. Evaporation, concentration, and dilution due to precipitation also affect the chemical composition of groundwater (Shikha & Singh, 2021). Kumar et al. (2006) stated that hydrogeochemical processes help to understand changes in groundwater quality due to water interaction with the host matrix and anthropogenic influences. The author further explained that groundwater quality depends also on the chemistry of water in recharge area and the geochemical processes that occur in the subsurface. Sharmin et al. (2020) also emphasized that these hydrogeochemical processes are responsible for the seasonal and spatial variations in groundwater chemistry. Industrial activities, mining operations, and agricultural practices are major culprits. Leaking landfills, improper waste disposal, and the use of metal–laden pesticides and fertilizers further contribute to the problem (Alfaifi et al., 2021; Sharmin et al., 2020).

Numerous methods and techniques have been applied to monitor, assess and spatially map groundwater quality to enhance water security of the groundwater–dependent communities (Masocha et al., 2019). Initially, assessments were mainly based on ground or field surveys, which involve routine field reconnaissance (Lekula & Lubczynski, 2019; Masocha et al., 2019). However, these methods are laborious, spatially limited, and costly, with the groundwater vulnerability to pollutants varying spatially and temporally depending on exposure levels (Masocha et al., 2019). It is, therefore, imperative to develop spatial explicit groundwater quality monitoring and assessment methods to help enhance the management of potential threats, hotspots and its use in general.

Statistical methods such as univariate and multivariate are used to characterise groundwater hydrogeochemistry in order to understand the dominant processes that affect its quality and assess its suitability for drinking and irrigation purposes. Principal component analysis (PCA) is a statistical method that is useful for interpreting and relating groundwater quality data to specific hydrogeological processes (Marghade et al., 2015). This method is rather useful for characterising and obtaining information of the groundwater system at a glance compared to going through complex methods and procedures (Krishan et al., 2023). In PCA, the degree of linear association between any two–groundwater quality parameters are measured by a value called correlation coefficient (Abdulsalam et al., 2022; Liu et al., 2020). Based on the PCA results, factor analysis can significantly explain observed relations among several variables in terms of simple relations that provide insight into the underlying structure of the variables (Matalas & Reiher, 1967). These simple relations are expressed in terms of a new set of variables, called factors. In the PCA, there is no prior knowledge about which sample belongs to which cluster. Linear regression is the next logical step in a bivariate hydrochemical analysis and is used to predict the value of a variable (dependent) based on the value of another variable (independent) (Das et al., 2022; Masoud et al., 2022). This method is useful in identifying relationships with the different measured hydrochemical variables and predicting one from a set of another variable. Hydrogeochemical investigations involve multiple variables and more than one of these variables can be predicted using multiple variables. Such multivariate environment thus necessitates the use of another method known as multiple regression analysis (Masoud et al., 2022).

The advent of geospatial techniques and remote sensing coupled with advanced statistical analytical methods has since gained moment in groundwater quality and vulnerability assessments (Gnanachandrasamy et al., 2015; Masocha et al., 2019; Reyes–Toscano et al., 2020). Furthermore, in recent years, several studies (e.g., Knoll et al., 2019; McLean et al., 2019; Pollicino et al., 2019; Sarkar, 2019; Vanclooster et al., 2019) have applied statistical modelling techniques in groundwater monitoring and mapping. Such approaches are useful in understanding the hydro–geochemical evolution in fractured rock aquifers. These methods permit the manipulation of a wide range of diverse hydrochemical data and parameters which are Indicators of groundwater quality and the prevailing aquifer hydro–geochemical processes (Sánchez–Martos et al., 2001). However, the major challenge with most of these studies is that they routinely assess and monitor groundwater quality at sites where groundwater resources contamination or pollution has occurred such as areas that experienced spillage of hazardous substances, or areas vulnerable to deterioration because of the perforation of aquitards (Bonte et al., 2015). Although such studies provide insights on groundwater status and quality across different scales, most of them fall short by failing to integrate a series of hydrochemical variables to determine the chemical evolution of the water especially in fractured acquires (Hussein, 2004; Sánchez–Martos et al., 2001). Thus, the main objective of this study was to determine groundwater quality of the fractured rock aquifers in the Beaufort West of the Karoo area using multivariate analysis and geospatial methods that utilise hydrochemical data. Multivariate (i.e., correlation and factor analysis) were used to characterise the hydro–geochemistry of the groundwater in order to understand the dominant processes that affect the groundwater quality and geospatial techniques were also integrated to determine the spatiotemporal variability of groundwater quality parameters.

2 Materials and Methods

2.1 Study Area

The study area was conducted in Beaufort West area (3203′1.70’’ – 32048′0.62’’ S latitude, 22016′12.85’’ – 23018′18.80’’ E longitude) of the Karoo basin of South Africa, about 460 km northeast of Cape Town. The fractured Karoo formation underlay the town’s location, which is heavily dependent on its groundwater resources for domestic, agricultural and industrial activities. The 48 boreholes in the study area are within six quaternary catchments (i.e., L11G, L12B, J21A, J21B, J21C, L11F) located within the two water management areas: Gouritz (primary catchment J) and Fish to Tsitsikamma (primary catchment L) (Fig. 1). The quaternary catchment J21A contains most of the borehole locations (Fig. 1). The spatial distribution of these boreholes is not uniform and is based on the local municipality’s groundwater abstraction plans. The cumulative mean annual precipitation (CMAP) of these catchments range from 165.6–229.9 mm, while the mean annual runoff ranges from 3.0–17.3 mm (Middleton & Bailey, 2011). According to the Groundwater Resources Assessment II (GRAII) report of the Department of Water and Sanitation (DWS) of South Africa, quaternary catchment J21A and L11F have mean recharge values of 1.76 and 2.32% of the total rainfall, respectively. This is equivalent to approximately 3.46 Mm^3/a and 3.79 Mm^3/a of mean annual runoff for these two quaternary catchments, respectively (Middleton & Bailey, 2011). Catchment J21A is densely populated with three major dams, recreational centres (e.g., swimming pools, golf estates), a wastewater treatment plant and commercially cultivated lands. The rest of the catchments are sparsely populated with most of them having non–perennial water bodies and commercially cultivated lands and game farms (Figs. 1 and 2a). The Karoo basin is a Late Carboniferous–Middle Jurassic retroarc foreland fill,

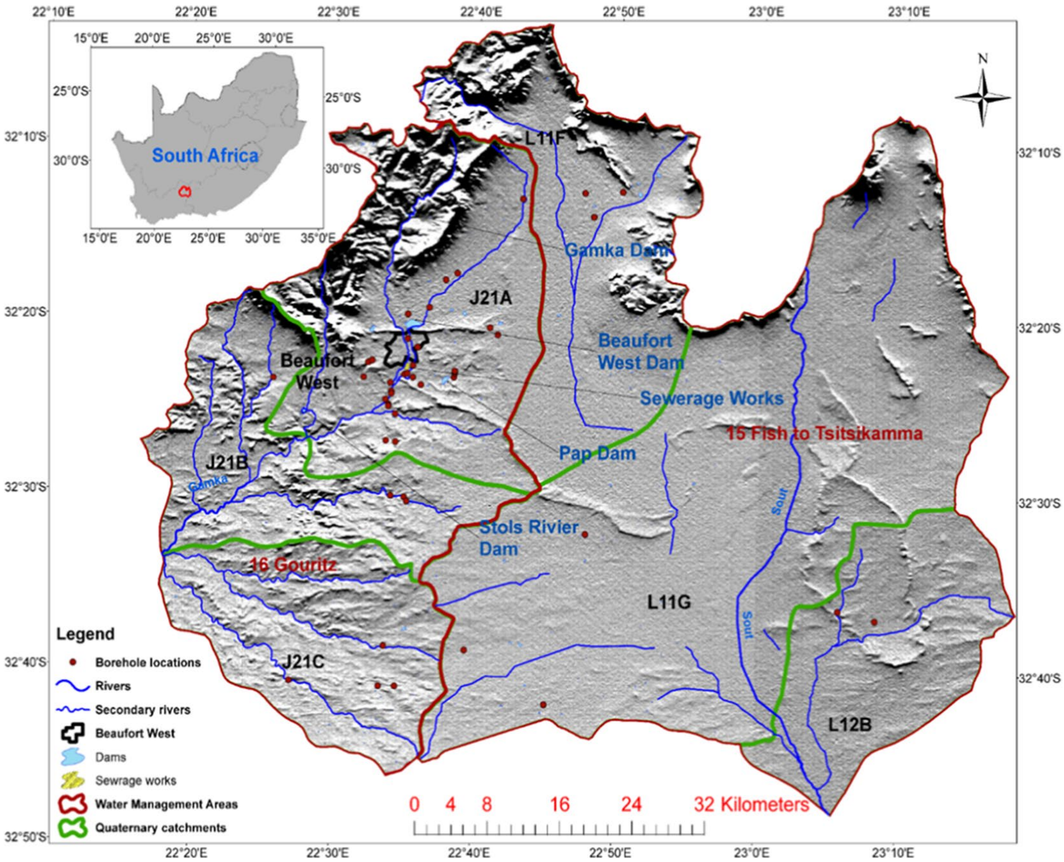

Fig. 1 Locational distribution of boreholes within the six catchment areas

developed in front of the Cape Fold Belt in relation to subduction of the Palaeo–Pacific plate underneath the Gondwana plate (Catuneanu et al., 1998). The sedimentary rocks of the Karoo sequence reflect the progressively changing depositional environment of a combined total thickness of about 12 km of sedimentary strata which are capped by a 1.4 km thick unit of basaltic lava (Fig. 2b, c) (Woodford & Chevallier, 2002).

The local geology of the study area is characterised predominantly by the lower Beaufort group which comprises of the mid–Permian Abrahamskraal ormation (Pa – light green in Fig. 2b) and the conformably overlying Late Permian Teekloof Formation (Pt – dark green in Fig. 2b) (Rubidge, 1995) and Jurassic dolerite dykes and sills (Jd – dark red in Fig. 2b). The northern part of the study area is mainly plateau of the Nuweveld Mountains that rise up to 1 450 m above mean sea level and is covered mainly by erosion resistant dolerite intrusions (Figs. 1 and 2c). The town of Beaufort West lies at the base of the escarpment.

2.2 Groundwater Sampling and Analysis

According to the Beaufort West Municipality, the boreholes in the study area were drilled in the shallow aquifer (< 70 m deep) zone. The selected boreholes were both municipal and privately owned and supply water for domestic demand and agricultural uses. Water samples were collected according to the South African National Standards (SANS) 241 sampling methods (SANS 241, 2006) from 49 boreholes in and around the town of Beaufort West. Borehole water was run and/or purged for 2–3 min and the polyethylene water collecting containers were rinsed first with 10% hydrochloric acid (HCl) (Merck Life Sciences, Johannesburg, South Africa) followed by

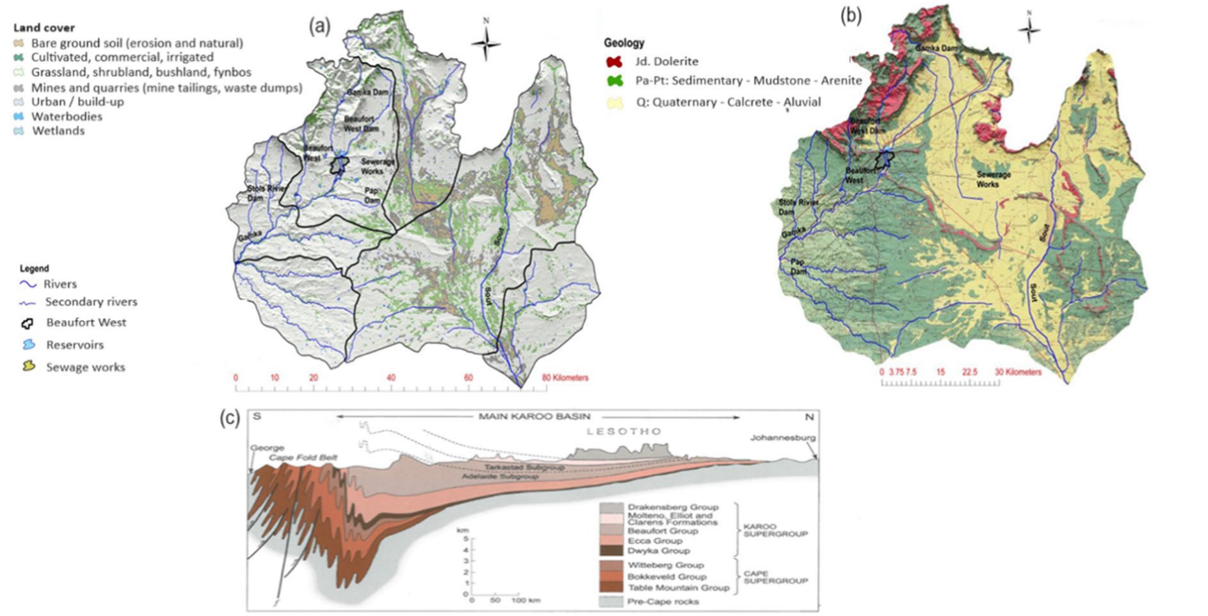

Fig. 2 (**a**) land cover and land use, (**b**) local geological map representation and (**c**) regional geology of the study area

deionized water and the sample water prior to sampling. On–site measurements of electrical conductivity (EC), pH, total dissolved solids (TDS) and temperature were done for all samples using portable handheld YSI multiparameter water meters (YSI Incorporated, Yellow Springs, USA). The cation samples were filtered with a 0.45 µm filter paper and acidified with nitric acid (HNO_3) (pH < 2) to reduce precipitation, adsorption to container and to accommodate possible trace metal analysis. The samples were sent to BEMLAB laboratory for major and trace elements analysis according to ISO/IEC 17025 standard. The hydrochemical parameters namely, calcium (Ca^{2+}), magnesium (Mg^{2+}), sodium (Na^+), potassium (K^+), bicarbonate (HCO_3^-), chlorides (Cl^-), sulphates (SO_4^{2-}), and nitrates (NO_3^-) were analysed. The Cl^- analysis was done by titration of the water samples with silver nitrate, while SO_4^{2-}, Na^+, Ca^{2+}, K^+ and Mg^{2+} were analysed using of inductively coupled plasma atomic emission spectroscopy (ICP–AES) (Shimadzu Scientific Instruments, Riverwood, USA). The HCO_3^- analysis was quantified by water sample titration with hydrochloric acid, whereas NO_3^- was examined using the cadmium reduction method and an auto–analyzer instrument before being determined spectrophotometrically. The reliability of the analysis results was determined using the ionic balance error of samples and 45 of them showed $\leq \pm 10\%$ error. The remaining four samples showed ionic balance error of ± 10–15% and these samples were included due to the relatively small number of the total samples.

2.3 Data Analysis

Hydrochemical variables of the groundwater samples were statistically analysed using multivariate statistical techniques. The degree of linear association between any two–groundwater quality parameters was measured using the correlation coefficient (r) value. Fourteen variables, the EC, sodium adsorption ratio (SAR), TDS, total hardness, total alkalinity, pH, Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^-, SO_4^{2-}, HCO_3^- and NO_3^- from the groundwater samples were analysed for their interrelation using Pearson correlation analysis.

Factor analysis of the natural log normalised groundwater hydrochemical data (i.e., Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^-, SO_4^{2-}, HCO_3^-, NO_3^-) was done to quantify the contributions of natural chemical weathering processes, ion exchange processes and anthropogenic effects on the measured ion concentrations. The factor analysis was done by computing the correlation matrix of the eight hydrochemical variables that involves the correlation coefficient (measure of interrelation). Correlation coefficients smaller than an absolute value of 0.20 were suppressed in this analysis. The factor loadings were then estimated and rotated to obtain easy interpretation of the resulting factors.

The principal component analysis (PCA) method was used as the parameter estimation method to transform the set of observed interdependent variables into an orthogonal set of variables called principal components (Matalas & Reiher, 1967). The resulting principal components accounted for the variance of the observed variables in such a way that the first component accounted for much of the variance and the succeeding components accounted for the residual variance not accounted for by the preceding components. The initial factor loadings obtained by PCA are, commonly, unlikely to reveal the underlying structure of the observed variables because of certain mathematical conditions, such as variance and properties of the principal component. To reveal this structure better, the common factor associated with the initial set of loadings were linearly transformed into a new set of common factors, associated with a new set of loadings, by factor rotation (Suk & Lee, 1999). Kaiser's scheme, called Varimax rotation, was used in this study to yield a set of loadings such that the variance of the square of the loadings becomes the maximum (Kaiser, 1958). In this study, the factor scores were obtained using the regression method (Johnson & Wichern, 2007).

2.4 Geospatial Techniques

The hydrochemical parameters were used to model the variability across the entire catchment in the GIS environment. The water management areas (based on drainage region boundaries), catchments (Quaternary catchment boundaries for South Africa) and other vector data were acquired from the Water Resources of South Africa, 2005 study (WR2005) (Middleton & Bailey, 2011). The water management areas and quaternary catchments of the study area were then extracted from these vector data. The Beaufort West 3222 raster map (Middleton & Bailey, 2011) and Shuttle radar topography mission (SRTM) elevation data of the study area were used to create orthorectified geological map. The raster map of the study area was extracted using the boundaries of the quaternary catchments that encompass the borehole locations.

Shuttle radar topography mission (SRTM) digital elevation model (DEM) for the study area was acquired from the United States Geological Survey (USGS) (NASA JPL, 2013). The South African National Land Cover vector data was obtained from the Agricultural Research Council of South Africa was used to derive land cover and land use information for the area under study. These vector files were analysed in ArcMap 10.6 (ESRI, Redlands, USA) and the area of interest was extracted using the boundaries of the quaternary catchments that encompass the groundwater sampling points. Some of the land cover attributes of these vector files were edited to simplify the display of legends created for land use maps. All the maps created in this study were projected using WGS_1984_UTM_Zone_34S projected coordinate system with the WGS_1984 datum.

Based on the spatial distribution of the boreholes, hydrochemical variables and multivariate statistical analyses results, different maps displaying major ions and factor analysis results against geology and quaternary catchments were generated. The spatial distributions of the major ions were spatialised using the inverse distance weighted (IDW), which is a deterministic interpolation (an exact interpolator) method. The IDW interpolation explicitly assumes that things that are close to one another are more alike than those that are far apart. This method assumes that each measured point has a local influence that diminishes with distance and gives greater weight to points closest to the prediction location (ESRI, 2020). This method was used due to the uneven distribution of the borehole locations and the objective was not to predict parameters accurately at unmeasured locations but rather provide a good way of looking at an interpolated surface for interpretation purpose. Thus, it doesn't provide prediction error assessment. A smooth search neighbourhood with a smoothing factor of one (that provides a maximum amount of smoothing by maximising the number of neighbours) was used to adjust the weights using sigmoidal function defined by the smoothing factor. Produced raster thematic maps were then displayed and classified using geometrical interval classification to accommodate the uneven distribution of the data. The factor scores were also displayed using the same methodology based on the display objectives.

3 Results and Discussion

The average pH of the groundwater samples was slightly alkaline, ranging between 6.6 and 8.3. The pH levels met the World Health Organisation (WHO) water quality limits for drinking water (WHO, 2017). The Ca^{2+} and Na^{+} had high concentrations, with mean values of 139.9 mg L^{-1} and 159.7 mg L^{-1}, respectively, while Cl^{-} and HCO_3^{-} were the dominant anion concentrations with mean values of 224.9 mg L^{-1} and 393.6 mg L^{-1}, respectively (Table 1).

The mean NO_3^{-} exceeded the South African Water Quality Guidelines (SAWQG) for drinking water target limit of 6 mg L^{-1} (Table 1). The standard deviations of the hydrochemical variables in general and TDS and Cl– in particular indicate that water in the study area is heterogeneous and reveals the influence of various contamination sources and natural geochemical processes. This variation could be attributed to differences in salinity and ionic composition (Kuldip–Singh et al., 2011).

3.1 Spatial Distribution of Ions

Groundwater chemically changes through its interaction with aquifer minerals, anthropogenic influences

Table 1 Groundwater hydrochemical variables measured from the 49 boreholes in the Karoo region of South Africa. All values are in mg L^{-1} except EC in mS m^{-1} and pH (no units). Abbreviations: Min. – minimum, Max. – maximum, std dev. – standard deviation, WHO – World Health Organisation, SAWQG – South Africa Water Quality Guidelines, EC – electrical conductivity, TDS – total dissolved solids, TA – total alkalinity, TH – total hardness, SAR – sodium adsorption ratio, Ca^{2+} – calcium ion, Mg^{2+} – magnesium ion, Na^{+} – sodium ion, K^{+} – potassium ion, HCO^{3-} – hydrogen carbonate, Cl^{-} – chloride ion, SO_4^{2-} – sulphate and NO_3^{-} – nitrate

Variables	Min	Max	Mean	Std. dev	SAWQG (DWAF, 1996) Target Water Quality	WHO (2017) recommended limit	Effect beyond target limit including mean values (SAWQG)
pH	6.6	8.3	7.51	0.41	6.0–9.0	6.5–8.5	
EC	56	477	170.3	92.8	≤ 70.0		Consumption of water does not appear to produce adverse health in the short term
TDS	424	3000	1202.3	614.3	≤ 450.0	1000	Water has marked salty taste and would probably not be used on aesthetic grounds if alternative supplies were available
TA	103.0	785.6	319.3	119.5			
TH	157.8	1733.8	514.5	304.3			
SAR	0.83	6.79	2.86	1.41			
Ca^{2+}	45.9	392.5	139.9	73.6	≤ 32.0	250	No health effects, severe scaling problems and lathering of soap severely impaired
Mg^{2+}	2.6	205.5	40.2	32.9	≤ 30.0	100	No bitter taste, slight scaling problems may occur and no health effects
Na^{+}	47.4	390.8	159.7	91.0	≤ 100.0	200	Faintly salty taste, threshold for taste and no health effects
K^{+}	0.01	30.57	5.39	5.12	≤ 50.0	12	No aesthetic (bitter taste) or health effects
HCO_3^{-}	125.6	950.8	393.6	149.0			
Cl^{-}	35.2	1088.7	224.9	205.8	≤ 100.0	250	Water has a distinctly salty taste, but no health effects. Likelihood of noticeable increase in corrosion rates in domestic appliances
SO_4^{2-}	14.9	954.5	211.3	184.5	≤ 200.0	250	Tendency to develop diarrhoea in sensitive and non–adapted individuals. Slight taste noticeable
NO_3^{-}	0.1	69.6	7.1	12.3	≤ 6.0	50	Rare instances of methaemoglobinaemia in infants; no effects in adults. Concentrations in this range are generally well tolerated

and internal mixing among different flow paths in the subsurface environment (Wallick & Tóth, 1976). Therefore, the spatial distribution of hydrochemical species provides information on the direction of groundwater movement. Solute concentrations in the groundwater increase due to spatial variability of recharge because of microtopographic controls (Schuh et al., 1997).

The spatial distribution of major ions Ca^{2+}, Na^{+}, Cl^{-}, Mg^{2+} and SO_4^{2-} in the study area (Figs. 3a–c and 4a, c) tend to show high concentrations on the alluvial sedimentary (calcrete) deposit (i.e., the northern part of the study area) compared to the lithofeldspathic sandstones of the Teekloof and mudstone arenites of the Abrahamskraal formations. This trend is also observed for Ca^{2+}, Na^{+} and K^{+} on the southern part of the town of Beaufort West, where the calcareous deposition is thin and combined with Teekloof formation (Figs. 3a, b and d). These high concentrations could be attributed to calcite dissolution, silicate weathering, ion exchange, evaporation processes and/or surface contamination in the northern and southern regions of Beaufort West. The surface contamination sources in these areas are mainly sewage and municipal effluents including urban and agricultural runoff (WHO, 2017). The concentration of the major cations (i.e., Ca^{2+}, Na^{+}, Mg^{2+}, K^{+}) is also high on the Teekloof formation where there is a contact with dolerite intrusions around Beaufort West compared to areas without any dolerite contacts (Figs. 3a–d). The dolerite intrusions increase the major cation concentrations in the groundwater through their contribution to silicate weathering. Low concentration of the above–mentioned cations and are mainly observed in areas where calcrete and the mudstone arenites of the Abrahamskraal formation dominate without dolerite intrusions.

In relation to the quaternary catchments, high concentration of the major ions, except for K^{+} was mainly observed in the J21A and L11F (Figs. 3a–c and 4a–c). These catchments have high cumulative mean annual precipitation (CMAP) (J21A – 229.86 mm and L11F – 219.75 mm) and increased weathering within the high lying areas compared to catchments

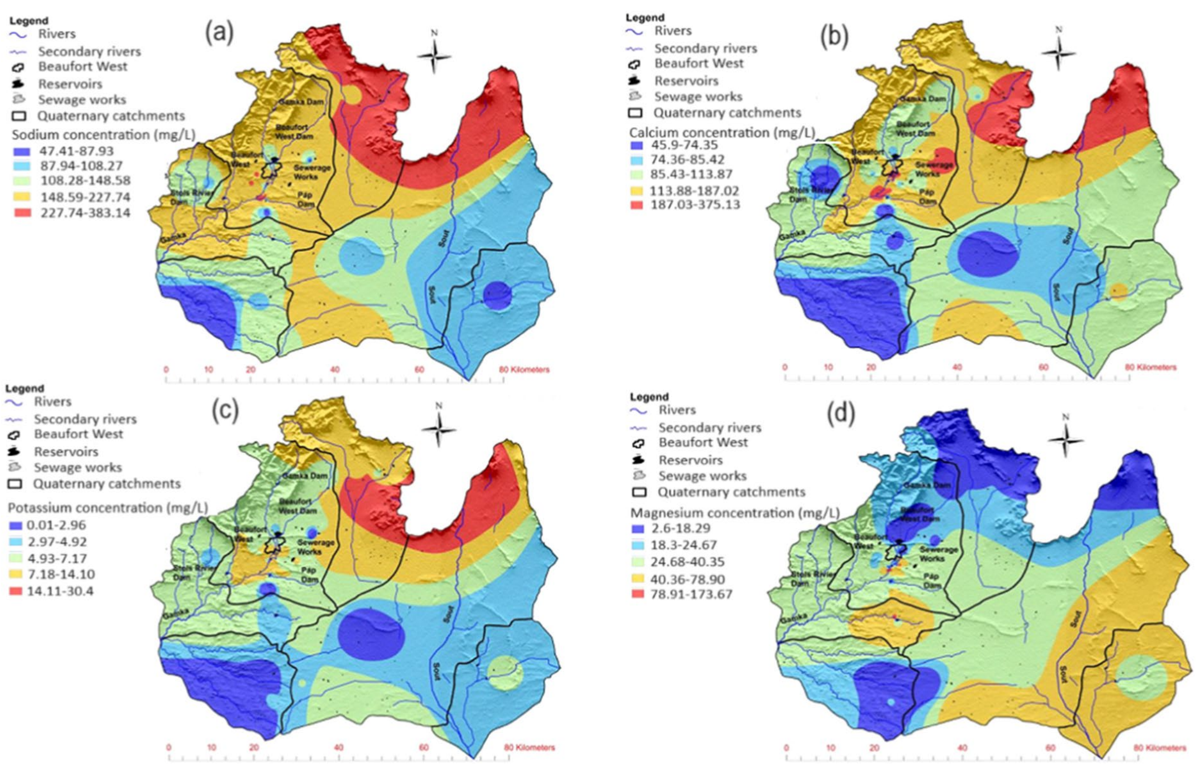

Fig. 3 Spatial distribution of (**a**) calcium (Ca^{2+}), (**b**) sodium (Na^{+}), (**c**) magnesium (Mg^{2+}) and (**d**) potassium (K^{+}) within the Karoo catchment areas across different lithological backgrounds

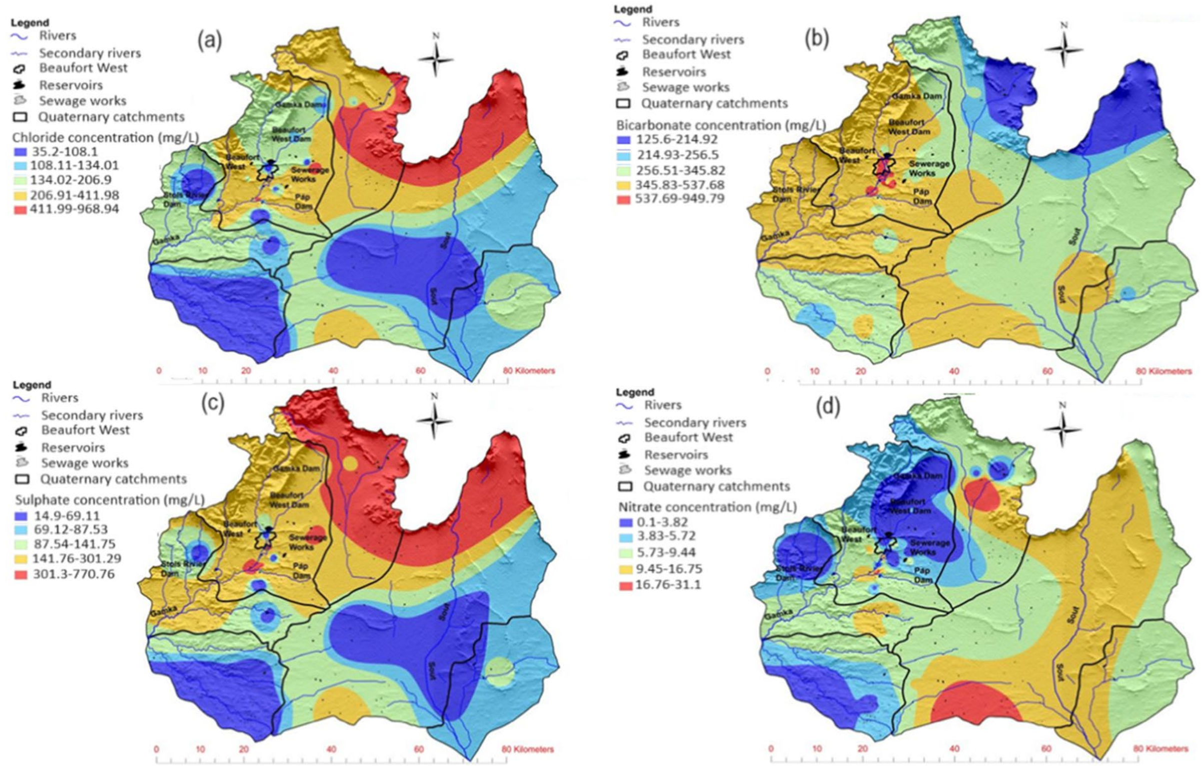

Fig. 4 Spatial distribution of (**a**) chloride (Cl^-), (**b**) bicarbonate (HCO_3^-), (**c**) sulphate (SO_4^{2-}) and (**d**) nitrate (NO_3^-) within the Karoo catchment areas across different lithological backgrounds

L11G, J21B, J21C and L12B. Having related the concentrations of these major ions to the rock formations and quaternary catchments, it can be inferred that the interaction with the lithology like the carbonates, lithofeldspathic sandstones and dolerites could result in high Ca^{2+}, Cl^-, Mg^{2+} and SO_4^{2-} concentrations due to dissolution and precipitation of evaporites and calcrete (Figs. 3a,c and 4a,c). The high Ca^{2+} and Mg^{2+} concentrations (Fig. 3a,c) were mostly recorded on the calcareous deposits on the northern part and south west of Beaufort West. These high concentrations could be attributed to the weathering and dissolution of calcite and dolomite in the calcrete, although Ca^{2+} is often the dominant ion in the calcite mineral (Parsons & Abrahams, 1994). The groundwater in these areas is characterised as hard. The Na^+ is distributed in a similar manner as that of Ca^{2+} and Mg^{2+} with high concentrations recorded on the calcrete deposits northeast, east, south and south–west of Beaufort West (Fig. 3b). These high concentrations could also be attributed to silicate weathering of the lithofeldspathic sandstones and ion exchange processes with some evaporation and halite dissolution. The Cl^- concentration distribution (Fig. 4a) is similarly high when compared to the Na^+ and Mg^{2+} concentrations (Fig. 3b,c) and could be attributed to surface contamination and halite dissolution. On the other hand, SO_4^{2-} concentration distribution (Fig. 4c) were similar to Ca^{2+} and Mg^{2+} concentration in the northern part of Beaufort West suggesting potential gypsum and/or anhydrite dissolution. To the south–west of Beaufort West, the SO_4^{2-} concentration distribution was high and could be ascribed to surface contamination besides sulphate dissolution. It was observed that the Cl^- and SO_4^{2-} concentrations in the J21A catchment's downstream (especially to the south) were high (Fig. 4a,c). These high concentrations were attributed to possible contamination from domestic waste and effluents from the sewerage works (Brindha & Kavitha, 2015; Fengxia Liu et al., 2019; Kumar et al., 2006).

The HCO_3^- concentrations (Fig. 4b) showed high concentrations mainly in the sandstones (basal arenaceous Poortjie Member) and mudstones areas of the sedimentary rocks. This could be attributed to the dissolution of soil limestone (which is predominantly calcite) in sediments during recharge. High concentrations were also observed in areas where there was sedimentary rock contact with dolerite intrusion. This observed high concentration in the dolerite contact zones could be the result of chemical weathering (carbonate dissolution and silicate weathering). A relatively low concentration is observed in the low–lying areas covered by the calcrete deposits. The J21A quaternary catchment recorded high HCO_3^- concentration compared to the other catchments.

The distributions of K^+ and NO_3^- concentrations across the six catchments are highlighted in Figs. 3d and 4d, respectively. In catchment J21A and J21B, K^+ and NO_3^- concentrations were high in areas with urbanisation, commercial farms, game farms and sewerage work (Fig. 2a). The high K^+ and NO_3^- concentrations observed in these catchments could be attributed to domestic effluents and agricultural contaminants (Arumugam & Elangovan, 2009), while chemical weathering and cation exchange processes in the lithofeldspathic sandstones of the Teekloof formation could also contribute to the observed high K^+ concentrations. Catchment L11F recorded low concentrations of K^+ (Fig. 3d) compared to NO_3^- (Fig. 4d). This contrast could be attributed to the contribution of synthetic fertilisers used in commercial irrigation and game farming resulting in high NO_3^- concentrations and is an indication of possible other sources of K^+. This is further highlighted by the negative correlation observed between these two cations (Table 2). The relatively high K^+ concentrations (Fig. 3d) in the agricultural catchments of J21C, L11G and L12B in comparison to that of NO_3^- (Fig. 4d) could be attributed to infiltration of K^+ into the groundwater from farm waste, animal feed and manure (Griffioen, 2001).

3.2 Relationship Among Hydrochemical Variables

Significant correlation for EC and the measured hydrochemical parameters were found to be highly positive correlated, with the exception of pH, K^+, HCO_3^- and NO_3^-. This indicated the role of rock water interaction in the chemical composition of the water in the Beaufort West (Kumar et al., 2006; Liu et al., 2015). The TDS was highly positively correlated with EC ($r=0.98$) (Table 2). Furthermore, TDS was significantly positively correlated to Mg^{2+}, Na^+, Cl^- and SO_4^{2-} in comparison to other measured ions and indicates that the hydrogeochemical process controlling their composition are partially related to those that control salinity (Gao et al., 2020). The strong correlation among the major ions Ca^{2+}, Mg^{2+}, Na^+,

Table 2 Correlation coefficient matrix of groundwater hydrochemical parameters from the Beaufort West region, South Africa. Symbols: * and † correlation is significant at $p<0.01$ and $p<0.05$. Abbreviations see Table 1

Parameter	pH	EC	SAR	Ca^{2+}	Mg^{2+}	Na^+	K^+	HCO_3^-	Cl^-	SO_4^{2-}	TDS	TA	TH	NO_3^-
pH	1													
EC	0.2	1												
SAR	0.26	0.56*	1											
Ca^{2+}	0.01	0.88*	0.27	1										
Mg^{2+}	0.12	0.90*	0.30†	0.82*	1									
Na^+	0.23	0.86*	0.88*	0.66*	0.63*	1								
K^+	0.35†	0.06	0.09	–0.0	0.04	0.07	1							
HCO_3^-	0.04	0.25	0.47*	0.05	0.09	0.46*	0.01	1						
Cl^-	0.15	0.95*	0.41*	0.86*	0.96*	0.73*	0.07	0.08	1					
SO_4^{2-}	0.21	0.92*	0.50*	0.84*	0.86*	0.77*	–0	0.04	0.89*	1				
TDS	0.14	0.98*	0.62*	0.84*	0.86*	0.89*	0.01	0.31†	0.91*	0.91*	1			
TA	0.01	0.24	0.43*	0.06	0.08	0.44*	0.01	0.99*	0.07	0.01	0.29†	1		
TH	0.06	0.93*	0.29†	0.97*	0.94*	0.68*	0.00	0.07	0.95*	0.89*	0.89*	0.1	1	
NO_3^-	0.05	0.27	0.13	0.31†	0.24	0.24	–0.0	0.04	0.27	0.15	0.24	0.1	0.29†	1

Cl^- and SO_4^{2-} with EC is an indication of the contribution of these elements to the salinity and permanent hardness of the groundwater due to concentration of ions from evaporation of recharge water, rock water interaction and anthropogenic activities (Brindha & Kavitha, 2015; Kumar et al., 2006; Liu et al., 2019). The permanent hardness (non–carbonate) is furthermore indicated by the strong positive correlation of total hardness to Ca^{2+}, Mg^{2+}, Cl^- and SO_4^{2-} in comparison to HCO_3^-, total alkalinity and pH (Table 2) (Liu et al., 2019; Reyes–Toscano et al., 2020). The strong correlation between SO_4^{2-} and Cl^- is also another indicator of the contribution of anthropogenic activities such as sewage discharge and irrigation to the water hardness (Liu et al., 2019).

Common K^+ containing minerals in sedimentary rocks include orthoclase, microcline, plagioclase, muscovite and other K–feldspars. The subsurface weathering of such silicate minerals and cation exchange processes are some of the possible sources of K^+ in groundwater and are affected by several factors including pH. The significant positive correlation of K^+ with pH (at $p < 0.05$ level) indicates potential infiltration source of this ion in comparison to temporary desorption source due to increased hardness (no correlation to total hardness, Table 2). The K^+ is generally depleted in groundwater because it is liberated with greater difficulty from the silicate minerals and high pH tends to increase the tendency of K^+ to be reincorporated into the solid weathering products. Thus, most of the K^+ in the groundwater samples (especially those from infiltration areas with agricultural land use) could be attributed to anthropogenic effect (farm waste, animal feed and manure spreading on calcareous soils) on the groundwater in the area (Griffioen, 2001).

Only factors with Eigenvalues ≥ 1 were taken into consideration and this resulted in three factors that were important and explained 81.4% of the cumulative variance. The variance explained by factor 1, factor 2 and factor 3 are 51.8%, 15.6% and 14.1%, respectively (Table 3).

The three factors shown in Table 4 were found to be dominated by certain variables based on the prevailing hydrogeochemical processes and land use practices. These three factors were named as "hardness", "alkalinity" and "anthropogenic" for factor 1, 2 and 3, respectively, based on the major contributing variables of the factor loadings, geochemical processes and anthropogenic activities influencing the groundwater chemistry (Table 4).

The main major ion contributors of the hardness factor were Cl^-, SO_4^{2-}, Ca^{2+}, Mg^{2+} and Na^+ (Table 4). This factor is ascribed to hardness and

Table 4 Factor analysis component loading result based on the rotation converged in 4 iterations. Extraction method: principal component analysis; rotation method: varimax with kaiser normalisation

Variable	Hardness	Alkalinity	Anthropogenic
Cl^-	0.96		
SO_4^{2-}	0.93		
Ca^{2+}	0.91		
Mg^{2+}	0.87		
Na^+	0.86	0.28	–0.22
HCO_3^-		0.85	–0.21
K^+		0.62	0.37
NO_3^-			0.92

Table 3 Total variance results from the factor analysis for the Beaufort West, South Africa. Abbreviations: var. – variance, cum. – cumulative

Component	Initial Eigenvalues			Extraction sums of squared loadings			Rotation sums of squared loadings		
	Total	% var	Cum.%	Total	% var	Cum. %	Total	% var	Cum. %
1	4.3	53.4	53.4	4.3	53.4	53.4	4.1	51.8	51.8
2	1.2	14.3	67.8	1.2	14.3	67.8	1.3	15.6	67.4
3	1.1	13.7	81.4	1.1	13.7	81.4	1.1	14.1	81.4
4	0.8	10.2	91.6						
5	0.3	4.3	95.9						
6	0.2	2.2	98.2						
7	0.1	1.3	99.4						
8	0.1	0.6	100.0						

salinity of the groundwater due to carbonate, silicate, gypsum and halite dissolution as well as infiltration of concentrated saline surface water resulting from evaporation and sewage discharges (Gao et al., 2020; Liu et al., 2019; Zhang et al., 2019). The high factor loading of Cl^-, SO_4^{2-} and Ca^{2+} on this component further explain the permanent water hardness in the study area. Figure 5 shows that the hardness factor score is high in the low–lying areas covered by calcrete deposits and the lithofeldspathic sandstones of the Teekloof formations near the dolerite intrusions to the south of Beaufort West.

The southern and south–western regions of Beaufort West had high hardness factor score distribution which could be attributed to surface contamination in addition to the rock–water interaction processes (Gao et al., 2020; Liu et al., 2019). The effect of fluctuating groundwater level coupled with rock water interaction results in the leaching of Ca^{2+} and Mg^{2+} from rock formations through the processes of carbonate and silicate weathering. The dissolution of these cations with Cl^- and SO_4^{2-} gives rise to the permanent hardness of the groundwater explained by significant ($p < 0.01$) positive correlation of TDS and total hardness to these ions in comparison to HCO_3^- (Table 2).

The Na^+ contributes the least to this factor compared to the other cations (Table 4) and had low correlation with Cl^- and SO_4^{2-} as compared to Ca^{2+} and Mg^{2+} (Table 2). This is an indication that this factor is of low salinity and high hardness due to a Ca–Mg–Cl–SO_4 type of groundwater chemistry. The low Na^+ loading on the hardness factor is also an indication of the influence of reverse ion exchange processes in conjunction with carbonate and silicate weathering in the groundwater samples characterised by this factor (Zhang et al., 2019). The hardness factor has high distribution in the J21A and L11F quaternary catchments (Fig. 5).

The alkalinity factor indicates the effect of alkalinity with HCO_3^- and K^+ being the major contributors (Table 4). This factor is related to carbonate and silicate weathering processes (Gao et al., 2020) and the observed high K^+ and low Na^+ loadings is attributed to alkalinity of the groundwater being dominated by K^+ due to cation exchange processes (Zhang et al., 2019). Total hardness normally depend on pH and

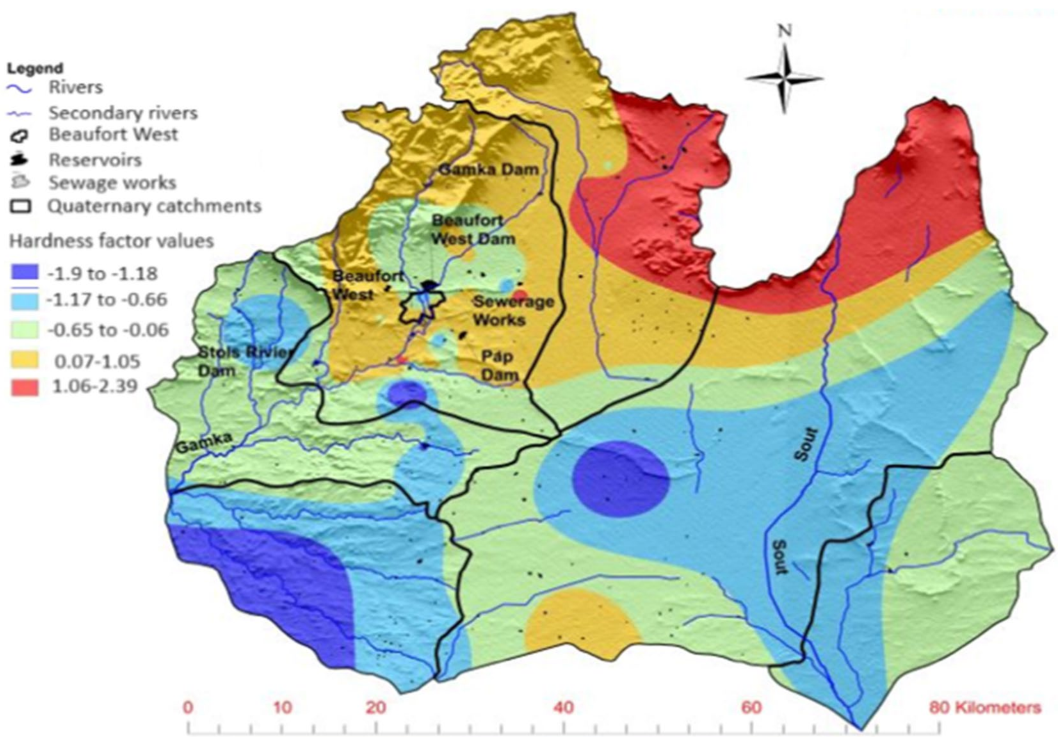

Fig. 5 Spatial distribution of the hardness factor scores within the Karoo catchment areas across different lithological backgrounds

total alkalinity since pH controls the hydrogeochemical process of groundwater. In this study there was a strong positive correlation between total hardness and HCO_3^- ($p < 0.01$), while these parameters lack any significant correlation with pH, total hardness, K^+, Ca^{2+} and Mg^{2+} (Table 2) and this could be a further indication of the effect of ion exchange (Reyes–Toscano et al., 2020).

The spatial distribution of the alkalinity factor presents high values in areas covered by the lithofeldspathic sandstones of the Teekloof formation especially in and around Beaufort West, where there is a contact with dolerite intrusion (Fig. 6). Low scores were observed in the low–lying calcrete deposit areas and the southern part of the study area. The J21A quaternary catchment shows high alkalinity factor scores compared to the other catchments (Fig. 6).

The anthropogenic factor indicates the effect of human activities on groundwater quality is dominated by NO_3^- and K^+. The J21A, J21B and J21C quaternary catchments, especially areas near wastewater treatment work and the informal settlements showed high anthropogenic factor scores (Fig. 7). Additionally, L11F, L11G and L12B quaternary catchments where both animal and olive farming are practiced show also high anthropogenic factor scores. High NO_3^- concentration can be also associated with recharge from precipitation and irrigation–carrying nitrogen compounds from soil into the aquifer. Non–agricultural sources of nitrate in the study area would include municipal and industrial discharges containing nitrogen bearing effluent and atmospheric deposition (Fengxia Liu et al., 2019).

3.3 Implications on Groundwater Quality

The integration of multivariate and geospatial technique tools in our research serves as a robust framework that can be emulated in groundwater quality assessments across geographical regions. Our findings shed light on some of the stressors affecting groundwater, as a significant portion of the groundwater samples analysed did not meet the drinking water quality guidelines. Given the low groundwater quality from certain boreholes, it is imperative to implement comprehensive treatment protocols

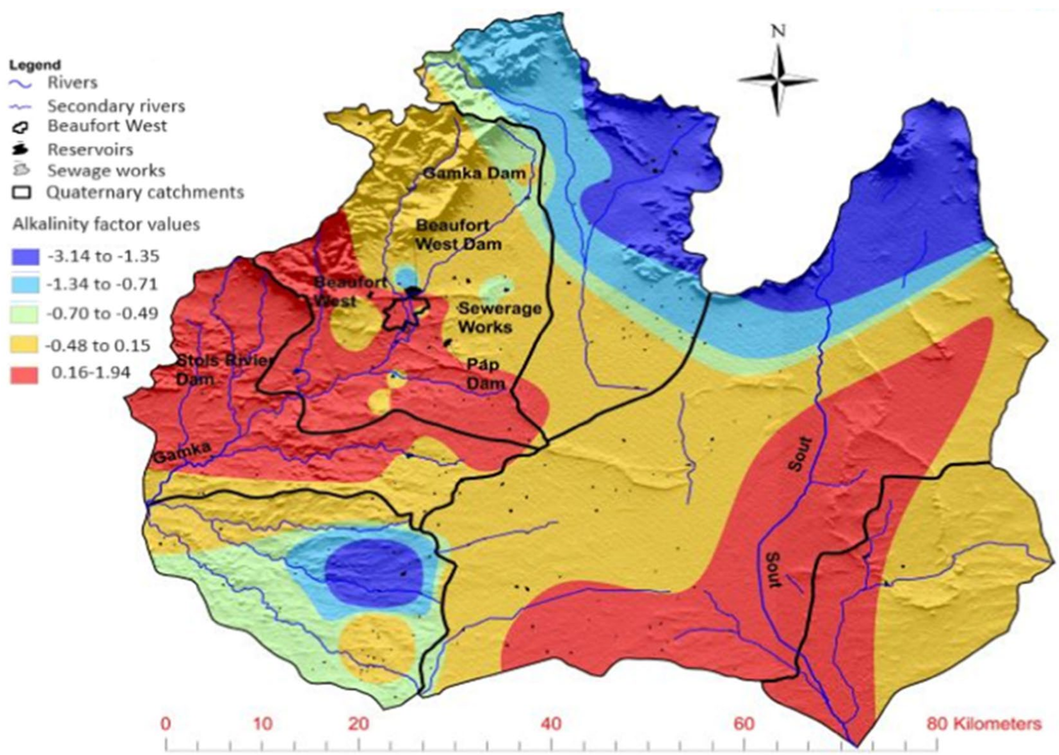

Fig. 6 Spatial distribution of the alkalinity factor loading within the Karoo catchment areas across different lithological backgrounds

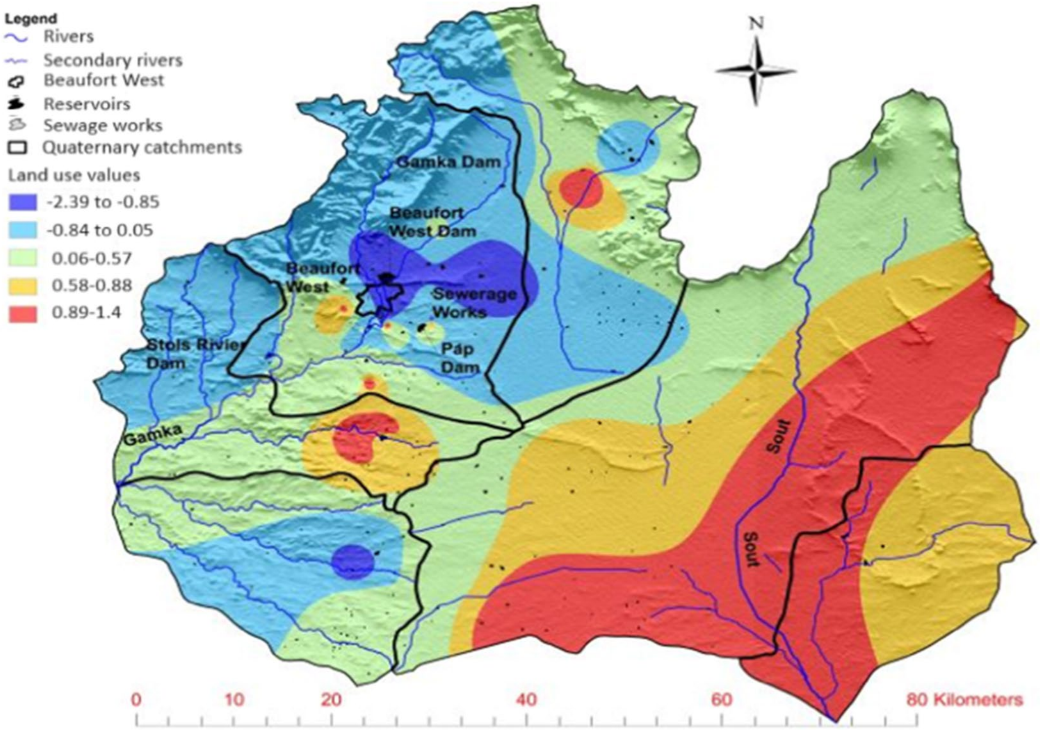

Fig. 7 Spatial distribution of land use (anthropogenic) factors within the Karoo catchment areas across different lithological backgrounds

to mitigate potential health risks associated with its usage. These treatment measures should be tailored to address specific contaminants identified, ensuring that groundwater supplied from these sources meets or exceeds regulatory standards for drinking water quality. In addition to treatment interventions, proactive strategies such as managed groundwater recharge initiatives are recommended to replenish aquifers and enhance overall water security. This underscores the urgent need for pre–emptive measures to ensure the safety and suitability of groundwater for domestic consumption. Furthermore, heightened monitoring efforts are warranted, particularly regarding groundwater extraction activities by private users, to prevent overexploitation and ensure sustainable resource management practices.

Identifying and addressing potential sources of groundwater contamination is paramount to safeguarding water quality. By pinpointing areas of concern and implementing targeted remediation measures, we can mitigate the risk of pollutants infiltrating groundwater sources. This necessitates a comprehensive approach that encompasses regular monitoring, stakeholder engagement, and the enforcement of regulations to prevent further degradation of groundwater quality. However, it's essential to acknowledge the limitations of our study, including the relatively small sample size and the uneven distribution of sampling points. To address these constraints and enhance the accuracy of our assessments, further investigations into the groundwater dynamics of the study area are warranted. A more strategically planned sampling approach, guided by hydrogeological principles, and informed by local conditions, will facilitate a comprehensive characterisation of aquifers and their water quality profiles.

4 Conclusions

The groundwater had a slightly alkaline pH, meeting both local and international drinking water quality standards. Hydrochemical parameters such as Ca^{2+}, Na^{+}, Cl^{-}, and HCO_3^{-}significantly influenced groundwater quality. Correlation analysis revealed that rock–water interaction, evaporation of recharge water, and anthropogenic activities contribute notably to water salinity and permanent hardness. Major ions showed high concentrations on calcrete deposits, while dolerite intruded lithofeldspathic sandstones of the Teekloof formation around Beaufort West exhibited increased concentrations of all major ions. Factor analysis elucidated three main factors, with factor 1 (hardness) which was primarily characterised by Ca^{2+}, Mg^{2+}, Na^{+}, Cl^{-}, and SO_4^{2-}, and accounted for the permanent hardness and low salinity of groundwater due to carbonate, silicate, gypsum, and halite dissolution, as well as infiltration of concentrated saline surface water from evaporation. Factor 2 (alkalinity) was characterised by HCO_3^{-} and K^{+}, while factor 3 (anthropogenic) was characterised by K^{+} and NO_3^{-}. These factors explained a significant percentage of the variance and exhibited spatial distributions similar to their contributing ions, suggesting influences from ion exchange, carbonate and silicate weathering, and precipitation of irrigation, municipal, and industrial discharges. Overall, these findings provide valuable insights into the hydrochemistry of the study area's groundwater, essential for effective water resource management and conservation efforts.

Authors Contribution HGS: Conceptualization, Methodology, Investigation, Data curation, Formal analysis, Funding, Writing – original draft, review and editing; TiD: Conceptualization, Methodology, Investigation, Data curation, Formal analysis, Supervision, Funding, Resources, Visualisation, Writing – original draft, review and editing; TD: Conceptualization, Visualization, Methodology, Investigation, Funding, Writing – original draft, review and editing.

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Data Availability All data has been presented in the manuscript.

Declarations

Competing Interest The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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