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Hydrogeochemical characteristics of groundwater in Latvia using multivariate statistical analysis

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The aim of this study is to determine geochemical processes denoting trace element levels and variations in the fresh groundwater in Latvia. The database of 1398 groundwater samples containing records about major ion chemistry, trace elements and geological conditions was made and used. Accuracy of groundwater analysis and errors were determined and excluded prior statistical analysis. Groundwater hydrogeochemical groups were distributed on the basis of major ion concentrations using Hierarchical Cluster Analysis (HCA) and Principal Component Analysis (PCA).

The results of PCA showed that there are three main geochemical groups explaining 84% of the total variance in data set. Component 1 explains the greatest amount of variance- 51% with main positive loadings of Cl, Na, K and Mg. Component 2 explains 21% of the variance with highest loadings of HCO_3, Ca and Mg. Component 3 shows the highest loadings of SO4 and Ca and explains 12% of the total variance.

HCA was chosen because of its great ability to group large amount of data (groundwater samples) in several clusters based on similar characteristics. As a result three large groups comprising nine distinctive clusters was made. It was possible to characterise each cluster depending on its depth of sampling, aquifer material and geochemical processes: carbonate dissolution (weathering), groundwater mixing, gypsum dissolution, ion exchange and seawater and upward saline water intrusion.

Cluster 1 is the least altered infiltration water with very low load of dissolved salts. It is concluded that the groundwater in Cluster 5 has evolved from Cluster 1 by carbonate weathering in an open system conditions. The Cluster 4 is similar to Cluster 5, yet have been affected by reduction of sulphates and iron species.

Cluster 3 is characterised by highest loading of chloride salts while Cluster 9 represents groundwater with highest sulphate concentrations resulting from gypsum dissolution. However, Cluster 8 is an intermediate product between the two previously named clusters. Groundwater in cluster 2, 6 and 7 is considered to be a result of carbonate weathering with some addition of sea salts or gypsum dissolution.

As a conclusion, the highest or lowest concentrations of some trace elements in groundwater was found out to be strongly associated with certain clusters. For example, Cluster 9 represents gypsum dissolution and has the highest concentrations of F, Sr, Rb, Li and the lowest levels of Ba. It can be also concluded that multivariate statistical analysis of major components can be used as an exploratory and predictive tool to identify groundwater objects with high possibility of elevated or reduced concentrations of harmful or essential trace elements.

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