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Assessing sustainable development of deep aquifers – Supplementary Information

Annette Dietmaier¹ and Thomas Baumann^{1*}

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¹*TUM School of Engineering and Design, Chair of Geohydrology, Technical University Munich, Arcisstr. 21, Munich, 80333, Bavaria, Germany.

*Corresponding author(s). E-mail(s): tbaumann@tum.de; Contributing authors: annette.dietmaier@tum.de;

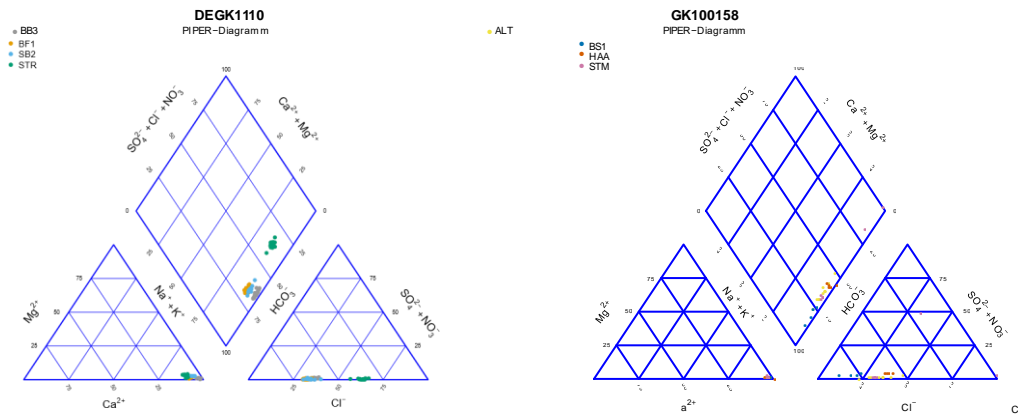


Fig. 1 Piper diagrams showing general hydrochemical composition of the assessed groundwater samples. Top graph shows wells in the GK100158 while those within DEGK1110 are displayed in the bottom graph.

Table 1 Result of mean and RSD values for TDS and each parameter when individual ions (Cl⁻, HCO₃⁻ and Na⁺) were left out in the clustering process in BF1. The top values are recalculated by Diana, the bottom values are recalculated by kmeans.

	All data	w/o Cl ⁻	w/o HCO ₃ ⁻	w/o Na ⁺
	Mean RSD	Mean RSD	Mean RSD	Mean RSD
	/mg/L/%	/mg/L/%	/mg/L/%	/mg/L/%
Na ⁺	Diana 295.650.03295.650.03301.260.02297.870.03			
	kmeans 295.650.03296.310.03308.010.02297.870.03			
K ⁺	19.840.2119.840.2117.750.1319.310.19			
	19.840.2119.740.2017.630.1319.310.19			
Ca ²⁺	21.110.1521.110.1521.180.1320.890.14			
	21.110.1521.200.1420.870.1020.890.14			
Mg ²⁺	3.520.303.520.303.870.253.670.26			
	3.520.303.570.283.850.253.670.26			
F ⁻	6.520.086.520.086.000.126.310.09			
	6.520.086.480.085.680.186.310.09			
Cl ⁻	162.570.04162.570.04166.390.04164.450.04			
	162.570.04163.610.04167.130.04164.450.04			
SO ₄ ²⁻	3.410.473.410.473.880.413.820.45			
	3.410.473.520.444.390.313.820.45			
HCO ₃ ⁻	593.470.01593.470.01606.850.02597.520.02			
	593.470.01595.290.01615.960.02597.520.02			
sum	1106.090.011106.090.011127.190.021113.840.02			
	1106.090.011109.710.011143.530.011113.840.02			

Table 2 Result of mean and RSD values for TD Sandea ch parameter when individual ions (Cl⁻ and HCO₃⁻) were left out in the clustering process in SB2. In contrast to BF1, the cluster structure did not change when excluding Na⁺, which is why the corresponding column is not shown in Table 2. The top values are calculated by Diana, the bottom values are recalculated by kmeans.

	All data w/o Cl ⁻	w/o HCO ₃ ⁻
	Mean RSD /mg/L/%/mg/L/%/mg/L/%	Mean RSD)
Na ⁺	Diana 276.640.03277.500.04279.140.02	
	kmeans 276.640.03274.730.03281.200.02	
K ⁺	15.920.0516.420.1315.800.04	
	15.920.0515.900.0515.620.03	
Ca ²⁺	12.800.1212.960.1313.000.11	
	12.800.1212.510.1213.600.06	
Mg ²⁺	4.380.024.420.034.380.02	
	4.380.024.380.024.380.02	
F ⁻	5.810.055.870.065.770.05	
	5.810.055.800.055.720.05	
Cl ⁻	157.930.05161.640.11158.930.05	
	157.930.05156.820.05163.100.03	
SO ₄ ²⁻	4.160.473.620.314.160.47	
	4.160.473.770.324.130.54	
HCO ₃ ⁻	547.150.02545.080.01544.770.03	
	547.150.02542.750.01546.300.03	
sum	1024.800.021027.520.031025.940.02	
	1024.800.021016.650.011034.050.02	

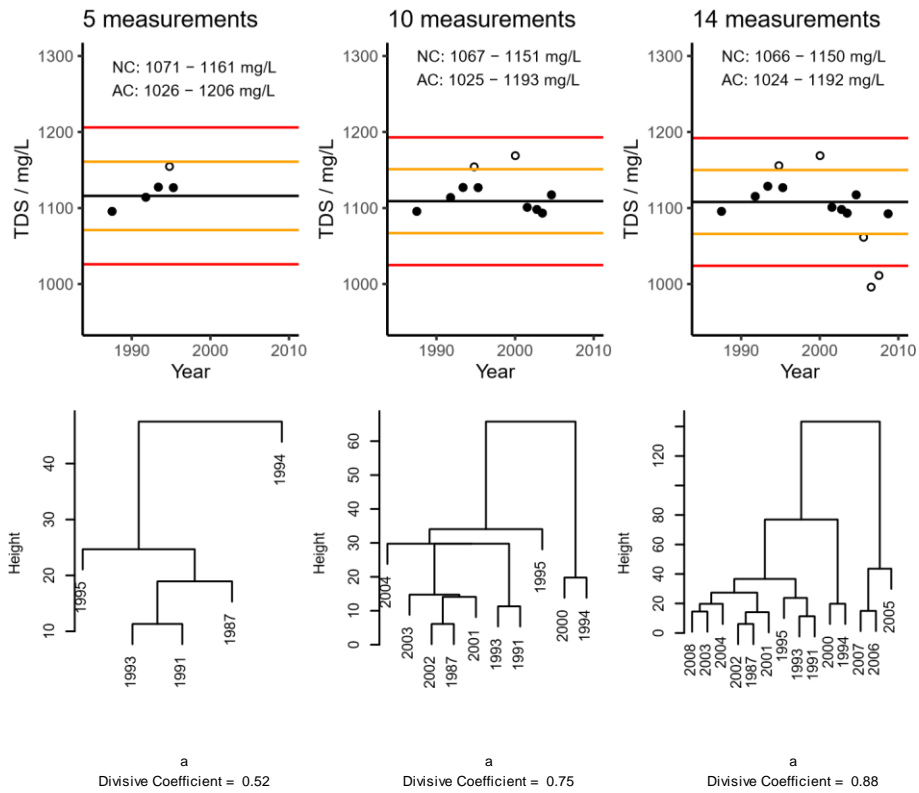


Fig. 2 Development of corridors with growing data set based on the Diana algorithm. The solid black dots represent the data points that were included in the main cluster.

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