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The Worth of Hydro Geochemical Data Factor Analysis (PCA) in Interpretation of Underground Water Origin. Megalopolis Lignite Bearing Fields Mine Water and Regional Waters Relations Case Study

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Abstract: In the region of Megalopolis basin (Peloponnese, South Greece), a number of lignite open pit mines are developed by Public Power Corporation S.A. in order to provide the electric power plants of 1200 MW with lignite. From environmental point of view is important to avoid negative effects of mines exploitation to significant regional ground and surface water reservoirs.

In this paper there was an effort to implement factor analysis in order to determine principal components on water analysis acquisition data in the region of Megalopolis Greece. The results of Principal Component Analysis (PCA) indicate two between five significant Principal components corresponding to samples collected from the internal mines dumping sites or pumping sites. The regional samples of water outside mines areas have factor scores insignificant to these two principal components.

Thus beside national legislation's and international standard limitations compliance that is company's environmental policy, PCA analysis confirmed the fact that there is no effect to the regional ground and surface water system by mine water.

Key words: Statistics, Principal Component Analysis, hydro chemistry

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1. Introduction

In Megalopolis lignite bearing basin a number of 4 open pit lignite mines have been developed in order to provide with lignite 4 power plants units of 850 MW. These mines are, Kiparissia, Thoknia(Fig. 1.), Marathousa and Choremi(Fig. 2.), mining fields.

In the region there are also sufficient groundwater and surface water reservoirs.

Alfios and Elissonas rivers flow between the mines (Fig. 1., Fig. 2.).

As artificial surface water bodies can be considered the ponds that have been created in the remnant Kiparissia field (PK1), in exhausted Thoknia mine (Pond 1 and II), the pumping site PM1 in Marathousa and the pumping sites into Choremi mine (P17-P27).

As far as it concerns the underground water the existence of two different types water bearing horizons is certified. One developed in loose sediments porous media of overburden and one in karstic system of basement and mountainous surroundings.

Today from the karstic system is pumping out 15-20 millions m^3 of ground water per year in order to cover the power plants cooling demands. This withdraw served also occasionally the hydrologic protection of Kiparissia mine from ground water inrush hazard till 2014.

From environmental point of view it is significant to avoid negative effects of mines exploitation to ground and surface water bodies.

The control of water quality was decided to performed based on the results of Principal Component Analysis interpretation, as it’s an international trend to environmental impacts investigations (Ting-Nien Wu, Chiu-Sheng Su, 2008).

2. Geological, Hydrogeological, Hydrological Conditions

In Megalopolis area the overburden consists mainly of low permeability marl and clayey material. In the system of loose sediments aquifers are formed very locally usually in gravels of old and recent riverbed deposits. Through these deposits the mines areas can be water recharged either by precipitation’s percolation or river’s water lateral inrush.

Around Thoknia mine field this overburden aquifer becomes a pure aquitard (Fig.1.). Basin’s basement and surrounding rocks are mainly karstified limestones. Into these karstified limestones different karstic aquifers are developed. The hydraulic connection between them is interrupted by flysch intercalations, mainly forming three karstic systems one west, one north and one main. This is certified on piezo metric measurements discontinuity. The most significant is the main Kiparissia karstic aquifer with 120 Km2 subsurface extend, 50

Km2 of which is surface appearance. Recharge is estimated 45% of precipitation (Chatzisavvas K., P.P.C, 2016) and mean annual precipitation is 900 mm. The termination of mine groundwater dewatering process in addition to successive reduction of pumping rates by power plants wells for cooling, result in an successive groundwater level appraisal.

Only on the floor Kiparissia mine is revealed an hydraulic relation between surface and subsurface karstic waters. There appears a contact of the karstic aquifer on limestone (BR, K, N, G borehole series), with the pit lake (PK1) which has been formed in Kiparissia mine after the end of the exploitation. Altitude of the lake surface, and consequently its depth and volume, is varying, following roughly the fluctuation of the karstic aquifer.

Ponds and permeable parts mine waste dumps that have been created in the remnant Thoknia mine (Pond 1-II), in Choremi mine (P17-P27), are hydraulic isolated from karst by impermeable marl formations under the bottom of the mine (Dimitrakopoulos, Vasiliou , Stathopoulos, 2016).

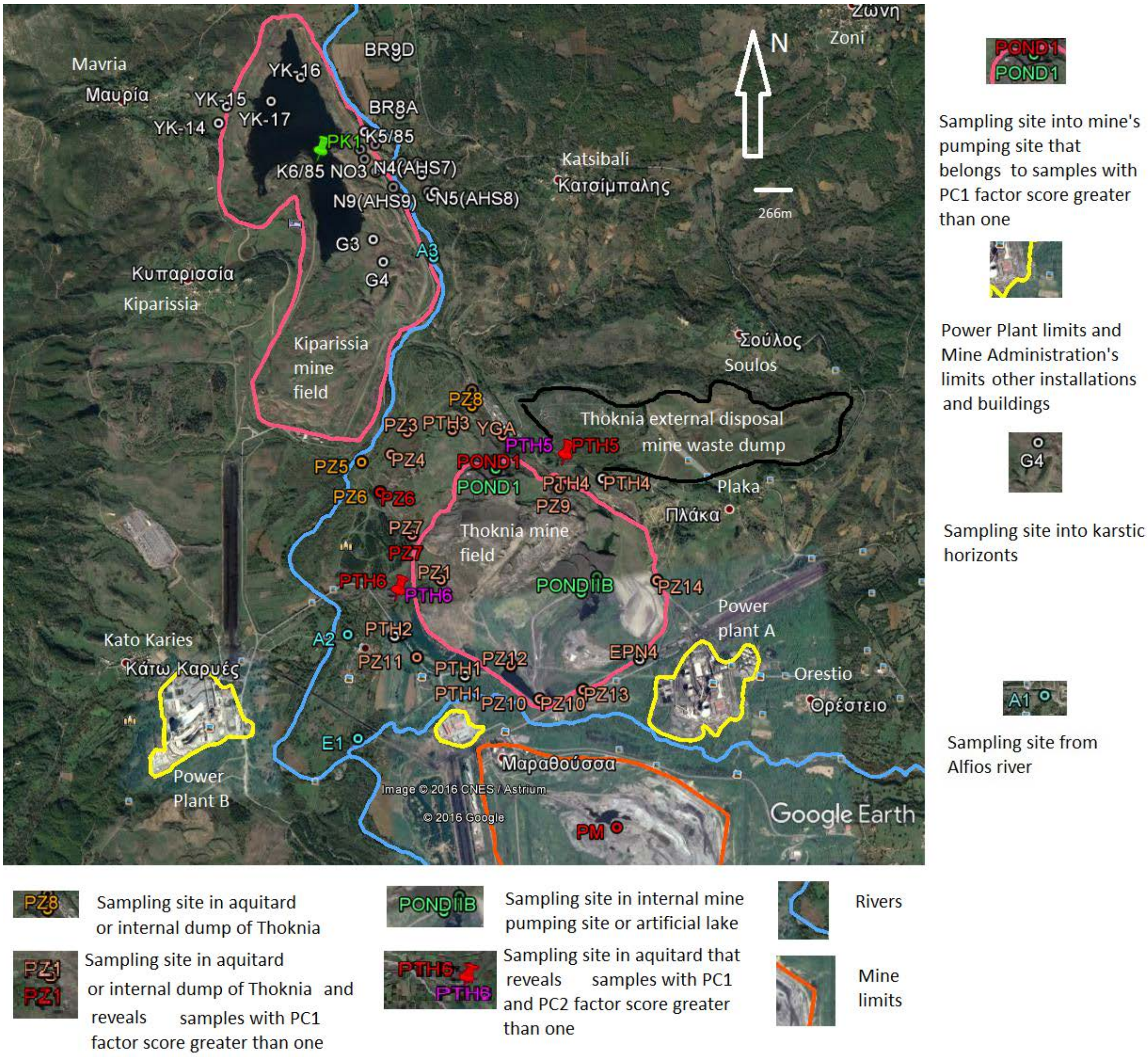

Figure 1. Sampling sites location map around Kiparissia and Thoknia mines. Samples of year 2015 characterization

3. Statistical analysis – Principal Component Analysis

In this presentation there was an effort to implement factor analysis in order to determine principal components of water analysis acquisition data in the region of Megalopolis Greece.

The primary data frame loaded as input in R language, was an initial matrix of 58 recent water samples that were collected, mainly during wet and dry season in 2015-2016. The chemical analyses of these samples on 17 hydro chemical parameters are performed by Center of Standards and Tests Chemical Laboratory of P.P.C. .

On the initial matrix A1-A6 are samples from Alfios and E1 from Elissonas River. Samples coming from the karstic aquifer (water wells named Br, K, N, G series) and from the poor aquitard around Thoknia mine (boreholes PTH, YGA, fig. 1.) were included.

Also additional 54 samples results of previous investigations (before 2015) (Dimitrakopoulou 2010; Waterchem 2007) concerning ground water quality were incorporated to the initial matrix.

P.C.A. was run in R-Studio source code.

This is a perfect example how useful can revealed in comprehension of underground water origin the use of principal component analysis (P.C.A.) in hydro geochemical parameters. As parameters can be considered basic element's concentration and physicochemical parameters records (T, pH, C.O.D., T.O.C. etc.). Each principal component corresponds to a group of parameters that contribute strongly to the total variance of data cloud.

Principal component analysis is based on matrices eigenvalues and eigenvectors theory.

First a basic principal component's (axis or factor) fingerprint determination, through its eigenvector, is accomplished. Then it is easy to distinguish by sample's factor score which of the samples have a certain relation between them according to an hydro chemical mechanism. The rest of the sampling cloud is considered not affected by this mechanism.

In Megalopolis hydro chemical data acquisition 4 basic principal components were identified PC1, PC2, PC3, and PC4 corresponding altogether to 76.5% of total cloud variance.

The eigenvectors of PC1-PC4 were evaluated as registered in Table 1. In the same table the standard deviation of each principal component and the percentage contribution of each axis to the total cloud variance are recorded.

The biplot of Principal Component analysis as far as it concerns the first two axis is depicted in figure 3.

The first principal component PC1 contains the parameters E.C., Ca, Mg, K, Na, Mn, NO_2^-, NO_3^-, SO_4^{--}, T.O.C. and C.O.D. with an increasing trend of all and in accordance with a pH decrease mechanism.

The samples that PC1 mechanism governs their origin, are the samples with PC1 factor score greater than 1.0. These samples are depicted in Fig.1. red marked.

All samples with PC1 Factor score greater than one, are collected from piezometers that are located mainly into Thoknia's internal deposit (PZ6,PZ7) and some pumping sites in Choremi, Marathousa and Thoknia as depicted in figure 1. and 2. sample location maps.

Factor score grater than 1.0 appears also in the aquitard (PTH5,PTH6 before 2016).

The PC1 samples corresponds to surface water from internal mine pumping sites or lakes. This water is enriched to elements water as it leaches the lignite desulphurization products rejected into the waste deposits or leaches lignite deposits itself.

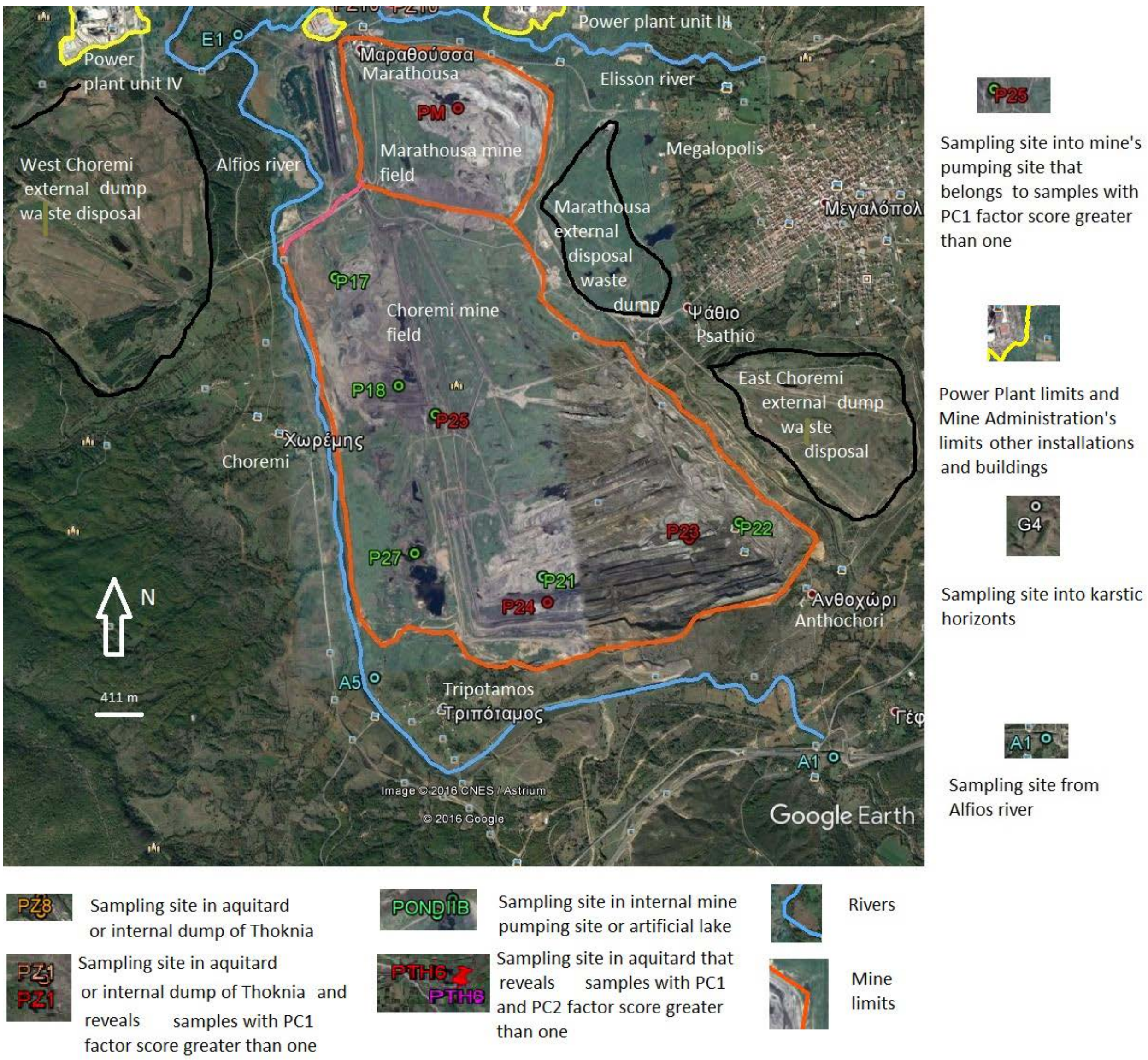

Figure 2. Sampling sites location map around Marathousa and Choremi mining fields. Samples of year 2015 charactirization

Apparently this mechanism is direct connected with the waste materials rejected and deposit mainly into the mine of Thoknia.

However no other sample is related with the above mechanism of PC1. The samples collected from Alfios river and karst groundwater samples in the broader region are not affected by the desulphurization products deposition. Even samples too close in Thoknia deposition region as YGA etc. are not ever related with PC1 mechanism.

The second component PC2 involves the parameters pH, SiO_2, Zn, HCO_3^{-}, Na^+ , SO_4^{--}, NO_3^- ions concentrations and corresponds to an hydro chemical mechanism that increase SiO_2, HCO_3^- and $N\alpha^+$,K^+ content while simultaneously decrease Zn^{++}, NO_3^-, pH, SO_4^{--} values.

The samples where the mechanism of PC2 dominates that have factor score greater than 1.0 in PC2(Fig.1.). These are mainly pumping site of Thoknia (pond1) plus only two samples (PTH5, PTH6 before 2016) of the aquitard near by Thoknia internal dump. No other sample have relation with this mechanism.

These samples corresponds to surface water from internal mine pumping sites or lakes and it’s an enriched to elements water as it leaches the lignite flying ash products rejected into the waste deposits.

This PC2 hydro geochemical mechanism is also related with a decrease of Zn^{++} mobilization , despite of pH decrease, when simultaneously concentrations of NO_2^- in NO_3^- are low. Such conditions appear in absence of agrochemical pollution (no fertilizers etc.) .

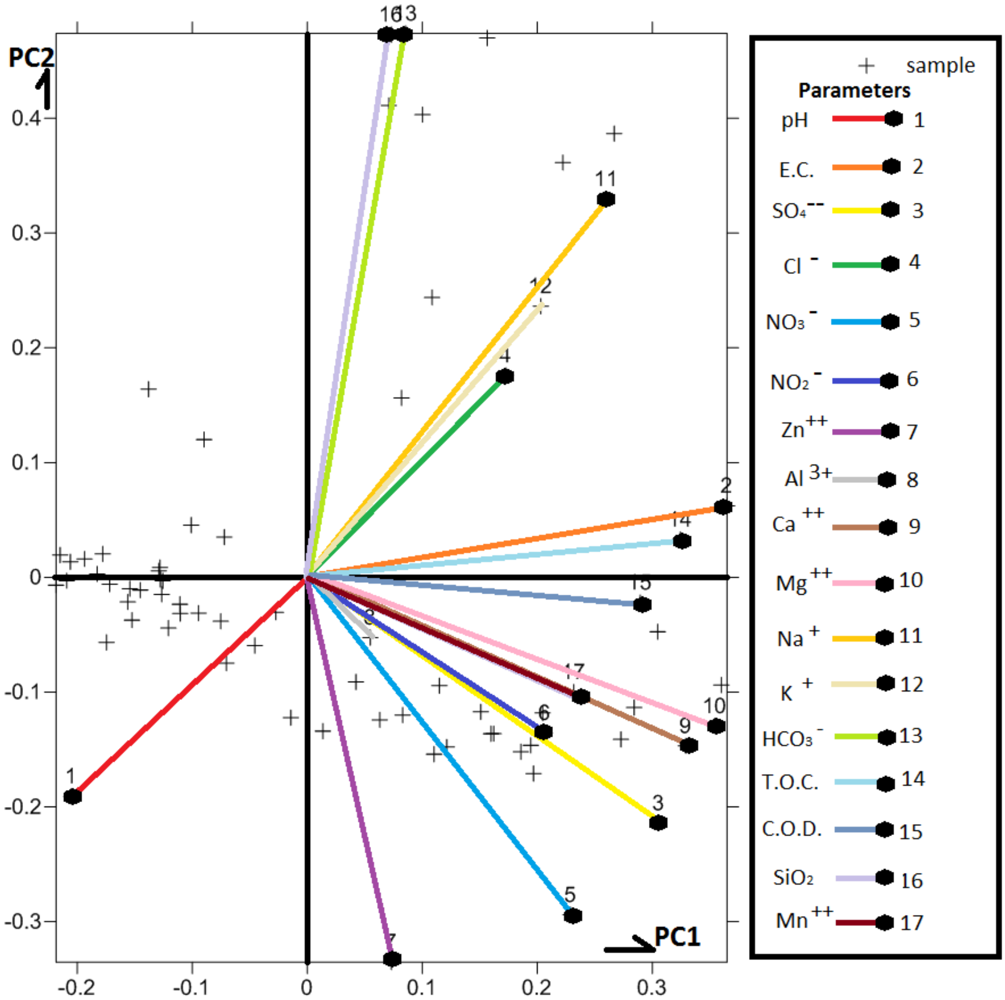

Figure 3. Biplot of samples and parameters on PC1 and PC2 components coordinate

In no sample of Alfios river this mechanism is significant. Is so insignificant that can be negible.

Alfios river water samples have no relation with this principal component and its mechanism.

Karst waters are also unrelated with PC1 mechanism.

The PCA also fact certifies the fact that borehole's YGA1, PTH water is in a great extend unrelated with the piezometer's PZ developed into Thoknia's deposition water.

The third axis PC3 contains the parameters pH, Al^{3+}, K^{+}, Mn^{++} and C.O.D., T.O.C. involved in a mechanism that values of their concentrations are increased drastically as the organic content (T.O.C., C.O.D.) and pH is decreasing.

No sample appears to have PC3 factor score greater than 1.0, coming to the conclusion that there is no sample affected by the large content K_2O, Al_2O_3 in flying ash.

The fourth axis PC4 contains the parameters pH, NO_2, T.O.C., C.O.D, Mn^{++}, Zn^{++}, Al^{3+} . involved in a mechanism that values of all concentrations and physicochemical parameters are increased drastically.

No sample appears to have PC4 factor score greater than 1.0.

The rest principal components seems to have no significance since each one have lower than 5% of total sampling cloud's variance.

Table1. Results of Principal Component Analysis – Factors Eigenvectors

Parameter	PC1	PC2	PC3	PC4
pH	-0.2051	-0.1908	-0.1857	0.3683
E.C.	0.3650	0.0623	-0.0153	0.0702
$SO4^{--}$	0.3057	-0.2143	0.1295	-0.0167
Cl^{-}	0.1727	0.1759	-0.1514	-0.1876
NO3-	0.2289	-0.2940	-0.1504	-0.0124
$NO2^{-}$	0.2064	-0.1355	-0.0887	-0.3566
Zn^{++}	0.0730	-0.3353	0.0982	0.4701
Al^{+++}	0.0547	-0.0524	0.6510	0.3784
Ca^{++}	0.3290	-0.1469	0.1197	-0.0012
Mg^{++}	0.3542	-0.1295	0.0278	0.0081
Na^{+}	0.2602	0.3297	-0.1568	0.1329
K^{+}	0.2030	0.2362	0.3435	-0.0494
$HCO3^{-}$	0.0856	0.4739	-0.0536	0.1822
T.O.C.	0.3243	0.0330	-0.2774	0.2303
C.O.D.	0.2894	-0.0220	-0.3387	0.2454
SiO2	0.0730	0.4729	0.1654	0.1320
Mn^{++}	0.2316	-0.0999	0.2860	-0.3849
Standard deviation	2.6653	1.9118	1.13019	0.98559
% of total variance	41.79	21.50	7.50	5.71
Sum % total variance	41.79	63.29	70.80	76.51

4. Conclusion

By applying the statistic method Principal Component Analysis to hydro chemical data we achieve two goals:

First PCA results became an alarm system that warns us for a leakage of polluted water before the logged parameters values reach the active values, following the next concept. If a sampling site sample traditional belonging to a group of natural regional water reveals an increase of sample's factor score to a principal component indicating a group of mine water there is risk.

This is quite important because the legislation limits compliance by itself is not sufficient protection of aquatic environment especially while as the qualitative status reaches the legislation limits this status becomes irreversible.

Secondary PCA results offer us a fare system in evaluation of each anthropogenic pressure participation to the total pollution.

As far as it concerns the case study of Megalopolis basin after 2015, there is no regional samples of water outside mines areas having factor scores significant to mine water first three principal components (PC1, PC2, PC3). In fact the factor score values are so insignificant that can be considered negible. That means that karst water, surface water and aquitard's water are not affected by mine water.

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