

Quantitative Assessment of Mine Water Sources based on the General Mixing Equation and Multivariate Statistics

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Abstract

The paper presents a methodology of quantifying different sources of water in the overall water entering a mine. This quantification is based on the hydrochemical nature of waters from individual aquifers contributing to the resulting mine water mixture. In order to solve the general mixing equation, the software tool KYBL has been developed using an over determined set of linear equations (3–10 sources defined by 4–12 parameters). The latest version KYBL-7 is the result of the research cooperation between VSB-Technical University of Ostrava and Silesian University of Technology, Gliwice. Its computational methodology is generally based on the balances of selected components of mine waters in steady state conditions without considering chemical reactions.

The methodology was applied in the Sokolov Coal Basin which is situated in the immediate vicinity of Carlsbad (Karlovy Vary), a worldwide renowned spa in the northern part of the Czech Republic. Both, the technology and coal mining methods used in the Sokolov Coal Basin are limited due to the proximity to the Carlsbad thermal springs. Because of their social and economic significance these springs are protected and mine planning must consider the priority of those springs. Consequently, the proportion of the Carlsbad type waters in mine waters of the Sokolov Coal Basin had to be evaluated.

Calculations proved that the contribution of the Carlsbad waters to the mine water is in the order of 3%. The imbalance in the mine water mixture using know source waters was quantified by including an 'unknown source' in the mixture simulation. Geochemical modeling demonstrated that the water quality is a result of geochemical reactions of waters in contact with the atmosphere and the reverse dissolution of the accumulated precipitates in the open pit areas. Those results have been used to assess the future technical measures that can be taken to protect the Carlsbad thermal waters.

Keywords Mine water sources proportions, open-pit coal mining, mixing equation, geochemical modeling, spring flow, water balance, Carlsbad/Czech Republic.

Introduction

Open-pit mining, whether during the active mining period or after closure, might significantly impact the rainfall-runoff conditions in quantitative and qualitative terms. Several of those impacts on the hydrological and hydrogeological conditions during the individual phases of mining activities are summarized in Younger et al. (2002) and Wolkersdorfer (2008). Open-pit dewatering typically induces a decline in groundwater levels (e.g. Younger 1993, Wardrop et al. 2001), changes in hydraulic gradients, leakage between aquifers, and induced inflows from adjacent aquifers. As a result, conflicts of interests tend to arise in ecologically sensitive areas, such as groundwater dependent ecosystems (Younger et al. 2004, Wolkersdorfer and Bowell 2005).

The Sokolov Coal Basin is situated in the immediate vicinity of Carlsbad (Karlovy Vary), the worldwide renowned spa, founded in 1338 by Bohemian King and Roman Emperor Charles IV. A total of 32 springs have been identified, thereunder 12 main springs producing 2000 L/min of mineralized water with temperatures between 35 °C and 72 °C (Vrba 1996, Laboutka and Vylita 1983, Paces 1988). Due to the presence and the social as well as economic significance of the springs, the technology and coal mining methods in the Sokolov Coal Basin must ensure that the springs are not negatively impacted. Especially because the geohydrodynamic system of these springs lies within a Graben structure (the Eger Graben Rift), there is a potential risk of the mining activities impacting the natural barriers.

In the past, several inrushes of gasified thermal waters into the mines have been observed: 1876 and 1881 in the Marie II Mine and another inrush in 1898 with up to 4,200 L/min (Hynie 1963). In all cases, the yield of the Carlsbad thermal springs began to fall. In 1908, after an inrush in the years 1906 (Hynie 1963), the total yield of the springs was by about one third lower than before and the CO₂ content of the Carlsbad spring water decreased as well. Even though recently the pumping tests failed to prove any direct relation to the Carlsbad thermal springs (Sokolov Coal Company, unpublished results), the drop in the springs' yield obviously occurred due to the degasification of the aquifer in the deeper granite massif. The measures undertaken to prevent the water inrushes to lately abandoned underground mines by grouting have been described by Kipko et al. (1993).

Mine water inrushes have an impact on occupational safety. Consequently, the quantification and forecasting of mine water inrushes are covered in a variety of studies (e.g. Keqiang et al. 2011, Zhu et al. 2008; Singh 1986; Vutukuri and Singh 1995). There are, however, not many studies dealing with methodologies to determine the ratios of mine water originating from individual aquifers (e.g. Perry and Evans 1999, Usher et al. 2010). Impacts of mine dewatering and inflows from individual aquifers tend to be analyzed by means of mathematical modeling (such as for the Wienclaw Lignite Mine: Koda 2008, Rapantova et al. 2007), or more generally by means of mathematical methods (Singh and Atkins 1985). The prediction of mine water discharges based on the least square vector equations (Xiaohui and Xiaoping 2010) or the combination of a numerical hydrogeological model with a lumped hydrological balance model to predict mine inflows (Sena and Molinero 2009) are examples of such solutions.

In the case of numerical models, the inflows from the individual aquifer systems form an indirect result from the model, based on the calibration targets of hydraulic heads achieved, the estimated hydraulic conductivities of aquifers, and the total dewatering rate. Knowledge of the proportional inflow rates from the individual aquifers may also facilitate the prediction of the trends in chemistry of the waters from the open pit dewatering and is dependent on the mine flooding rates and/or on the climatic influences.

Direct measurement of mine water flows requires the use of hydrometric techniques for measuring the flow rates of springs, streams, and rivers. Those techniques are well established and widely described in the literature (e.g. Brassington 2006; Wolkersdorfer 2008) with particular methods used in the mining conditions (PIRAMID Consortium 2003). Yet, many measurements tend to have a considerable degree of uncertainty given the potential diffuse flows – if they are feasible at all. Investigations in selected mines showed that many flow measurements must be considered wrong because the prerequisites of the individual methods were not accurately taken into consideration (Wolkersdorfer 2008).

The objective of this paper is presenting an alternative indirect method of calculation the proportions of mine water inflows into a mine water sump. The calculations and the quantities of the various water resources contributing to the total mine water mixture are based on the hydrochemical data from groundwater in individual aquifers and the chemical composition of the mine water in the dewatering sump. To solve the general mixing equation as an overdetermined set of linear equations (3–10 sources defined by 4–12 parameters), the KYBL-7 software has been developed (Krzyszowski et al. 2005) and will be discussed in detail in the section 'Methods'.

The basic philosophy of calculating the proportions of water sources in a mine water mixture used by KYBL is very similar to that in the code M3 (Multivariate Mixing and Mass balance calculation) created within the Äspö Hard Rock Laboratory Research Programme (Laaksoharju et al. 1999, Laaksoharju et al. 2008). Both codes utilize hydrochemical data for calculation of the proportion of the water sources in the mixture including 'sources and sinks' identification. Nevertheless, the mathematical methods applied are very different. M3 uses Principal Component Analyses (PCA) to summarize the information from the data set and further modeling. M3, as declared by the authors, should be used if two principal components of the data set sum up to more than 60% of the variability or the information in the data set. This assumption is quite often met in data sets. The tested margin of the model is $\pm 10\%$ for the Äspö site data (Laaksoharju et al. 1999) but depends on the tested data. A mixing portion of less than 10% is regarded as under the detection limit. Gómez et al. (2008) presents a study concluding that the robustness of the output of M3 is quite sensitive to whether only conservative compositional variables are used or both conservative and non-conservative compositional variables. According to this study, mass balance calculations in M3 are much more sensitive to non-conservative compositional variables and the recommendation here is not to use non-conservative variables with PCA-based codes if any information about reactions is to be obtained.

Another program that is commonly used to compute proportions of source waters contributing to final mixed water is NETPATH (Plummer et al. 1994). This inverse geochemical modeling code takes into consideration 2 to 5 initial solutions. Based on a set of analyzed parameters and a user defined selection of mineral phases a number of potential mixing models is calculated based on chemical thermodynamic calculations. In addition to the mixing, dilution and evaporation processes can be modeled. NETPATH has an export function to PHREEQC and the advantages of PHREEQC can be used in conjunction with NETPATH to model mixing scenarios of known sources. However, the alternative inverse modeling approach of PHREEQC results in many sets of mixing proportions and mineral mass transfers. Consequently, the use of this methodology becomes very difficult and tedious when applied to large groundwater datasets (Gómez et al. 2008).

We will exemplify the application of the software tool KYBL (Czech word for bucket, used in mine shaft construction) by using a case study from the Sokolov Coal Basin. Our aim is to quantify the mine water inflows from individual aquifers and identify the proportion of the Carlsbad type mineral waters. Based on the results, the technical measures taken to protect the Carlsbad thermal waters system have been assessed.

Geological and hydrogeological conditions

The Sokolov Coal Basin is part of the Podkrusnohorské Basin belonging to the Tertiary Eger Graben Rift (Kopecký 1978, Adamovic and Coubal 1999, Cajz and Valecka 2010), which hosts also thermal springs in its eastern part (Dupalová et al. in press). According to Ziegler (1990), the Eger Graben Rift is part of the European Cenozoic Rift System (ECRIS; Rajchl et al. 2009), a large tectonic-sedimentary system in Central Europe, characterized by its Cenozoic sedimentary basins and intense intratubular alkali volcanism. Neovolcanism took place during the evolution of the rift structure with the main volcanic centers and intrusions following cross fractures with a prevailing NW—SE orientation. Those intrusions resulted in the dividing of the Eger Graben valley into separate sedimentary basins with the Sokolov Coal Basin being one of those (Fig. 1).

Within the Eger Graben Rift, the Sokolov Coal Basin is of particular importance in this study, as its basement is mostly composed of the Carlsbad Pluton granites. Due to its tectonic structure, the Sokolov Coal Basin can be divided into a series of blocks (Rojik 2004) with the Carlsbad fracture and the “hot springs fracture” zones being of particularly significance relating to the Carlsbad mineral water genesis (Mísař et al. 1983).

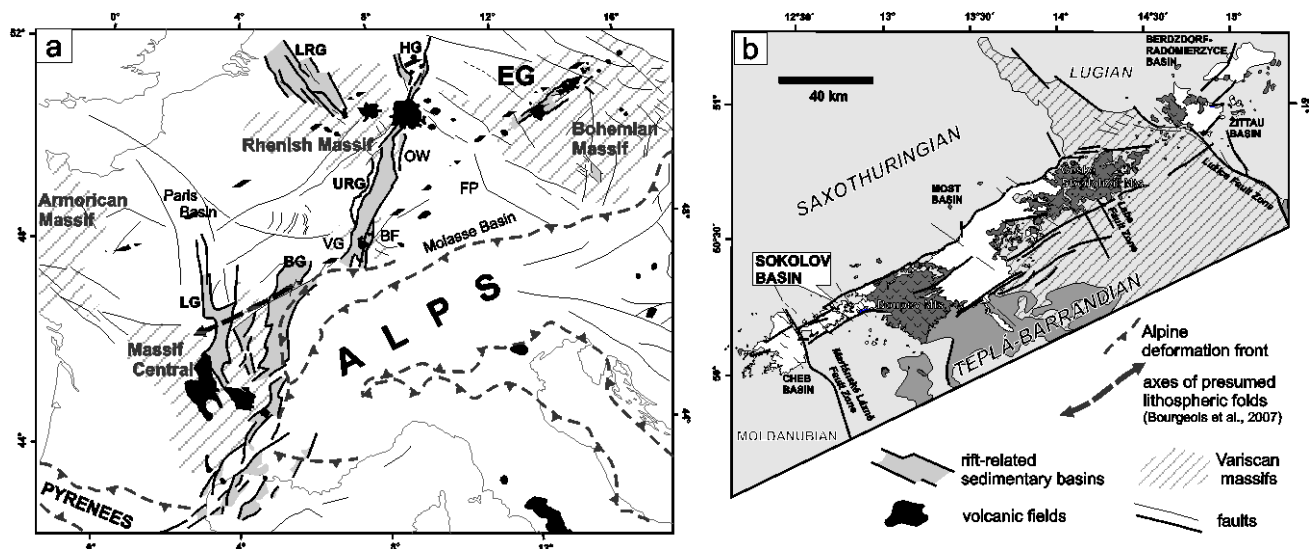


Fig. 1 (a) Schematic map of the Eger Graben as a part of the European Cenozoic Rift System (ECRIS; modified after Dézes et al. 2004; BF: Black Forest. BG: Bresse Graben. EG: Eger Graben. FP: Franconian Platform. HG: Hessian grabens. LG: Limagne Graben. LRG: Lower Rhine [Roer Valley] Graben. OW: Odenwald. VG: Vosges) (b) Schematic geological map of the Eger Graben with the location of individual sedimentary basins and volcanic domains (after Rajchl et al. 2009)

Depending on the water chemistry and pressure conditions, the Sokolov Coal Basin’s aquifers can generally be subdivided into the upper Tertiary aquifers (Cypris Formation) and basal aquifers (Old Sedlec Formation Aquifer, Josef Seam Formation, crystalline basement aquifer; Homola and Klir 1975). Mine dewatering strongly influences the ambient hydrological conditions around the open pit, because the large scale dewatering causes a drop in the groundwater levels in the surrounding Tertiary aquifers. In some areas, the dewatering reaches as deep as the basal aquifers below the Tertiary erosion base. Originally, the area was drained by surface watercourses, but the extensive dewatering has resulted

in a decrease in the baseflow, reaching beyond the limits of the area of interest due to the extension of the depression cone with a maximum drawdown of approximately 70 m. As a consequence of the changed hydraulic gradients toward the drainage centers, the runoff losses infiltrate through the tectonic faults and seams into the mine workings and open pits. In addition, the dewatering lowered the current regional groundwater levels below their natural levels before the dewatering took place. As described above, the mine dewatering has also reduced the hydraulic pressure in the deep groundwaters of the Old Sedlec Formation and the crystalline aquifers. In order to protect Carlsbad's natural curative resources, it was therefore necessary to investigate potential impacts around the basal aquifers of the Josef Seam Formation, of the Old Sedlec Formation, and of the crystalline basement aquifers.

According to Hokr (1961), the aquifers are recharged with groundwater of three types: (a) cold waters infiltrating mainly along the western edge of the Sokolov Coal Basin, (b) warm waters that rise in the upper parts of the granite pluton, infiltrated mainly on the slopes of the Krušné Hory Mountains (Ore Mountains), and (c) hot gassy mineral water springs, emanating in the deeper parts of the granite pluton. Though the warm water in the basal confined aquifer of the crystalline rocks has no direct relationship with the Carlsbad thermal springs, it is, however, demonstrably influenced by the leakage of thermal water through zones of lower hydraulic resistance. This is due to the higher piezometric level of the Carlsbad thermal springs which enables the waters to leak to the basal aquifer where higher hydraulic conductivities between the aquifer systems can be found. Moreover, this situation causes a temperature and hydrochemical heterogeneity within the basal aquifer water body.

Water intrudes into the mine along the local fracture zones are mainly controlled by two factors: the hydraulic pressure of the basal aquifer and the lower hydraulic conductivity of the underlying rocks. All pressure reductions under the bottom of the two active mines in the Sokolov Coal Basin (Jiří and Družba Mines; Fig. 2) must therefore be carried out in accordance with the measures taken to protect the Carlsbad thermal springs. Unfortunately, the dewatering of the basal aquifer significantly influences the conditions throughout the wide neighborhood of the active Jiří and Družba Mines as well.



Fig. 2 Pumping of gasified thermal waters in the Jiri Mine; Borehole OV-73 (photo: Galek)

Methods

Background

In order to protect the Carlsbad hot springs, it was necessary to quantify and determine the proportion of the Carlsbad type waters in the drainage water of the Jiří and Družba Mines. Those calculations, where proportions of various waters in a given water sample have to be calculated, are an essential problem in applied hydrogeology. (e.g. Kresic 1997, Fetter 2001, Gómez et al. 2008). In particular, the proportion of sources for a given water sample as well as the final composition of mixing waters of a known composition need to be known. Wolkersdorfer (2008) describes the results of such a calculation for the Gernrode fluorspar mine, where the numerical code PHREEQC was used to identify the ratio of mine water and mineral water discharging from the mine.

In case of the Carlsbad hot springs, these investigations were preceded by defining the hydrogeochemical compositions of the mine water sources by means of groundwater from monitoring boreholes data taken in the years 2004–2006. Multivariate cluster analyses were used to identify and visualize the hydrogeochemical data of the groundwater from the dewatering boreholes. Of the 127 water samples from boreholes, one sample from the Grasset Fault inrush (January 2003), and one sample from the Carlsbad hot spring (2006) ten parameters were used for the cluster analysis: total dissolved solids (TDS), Na^+ , K^+ , Ca^{2+} , Mg^{2+} , Cl^- , SO_4^{2-} , HCO_3^- , NH_4^+ , and Fe^{2+} . We applied PCA (Jolliffe 1986) in order to transform the original set of variables to a new set of uncorrelated variables and run hierarchical cluster analyses on both original and transformed data matrix with no important difference.

Cluster analysis was conducted with MATLAB using the Ward clustering strategy (Manly 1994). The code generates a dendrogram with similarity/dissimilarity values for samples and a computation log with information on the individual clusters (Cressie 1993). These results were used to define the relevant hydrogeochemical parameters of the source waters to calculate their proportions in the mine water mixture from the mine sump.

In order to quantify the proportions of source waters composing the Jiří and Družba mine waters, the previously developed numerical code KYBL-7 was used (Krzyszowski 2005, 2009, Krzyszowski et al. 2005). Its computational methodology is generally based on the balances of selected components of mine waters in steady state conditions without considering chemical reactions. Fig. 3 shows the conceptual model used to compute the waters mixtures by means of KYBL-7.

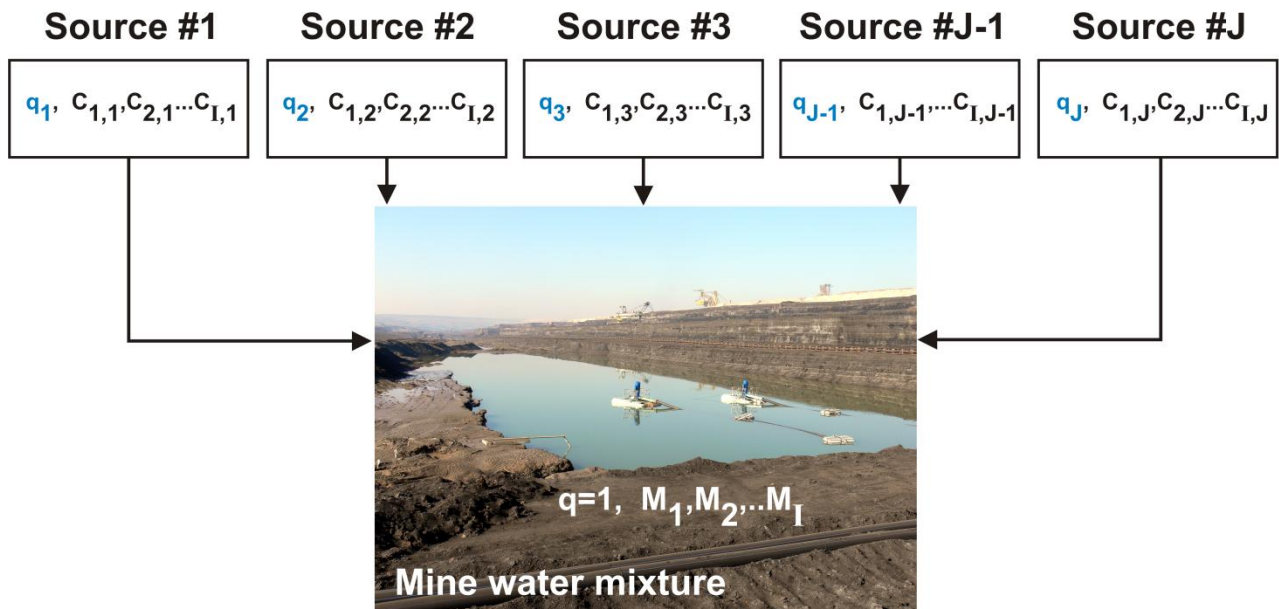


Fig.3 Diagram of the water mixture for J mine water sources with known compositions ($c_{i,j}$) and unknown proportions (q_j) in water mixtures with known compositions (q, M_i). Unknown variables, constituting the unknown quantities of the system are marked in blue

The mathematical equation to describe the fractions of the different source waters composing the mine water are based on the following equations:

$$\sum_{j=1}^J q_j \cdot C_{1,j} = M_1 \tag{1a}$$

...

$$\sum_{j=1}^J q_j \cdot C_{I,j} = M_I \tag{1i}$$

where:

$C_{i,j}$: concentration of the i -th component in the j -th water source: $i=1 \dots I, j=1 \dots J$).

M_i : concentration of the i -th component in the mine water mixture: $I = 1 \dots I$,

q_j : proportion of the j -th mine water source in the water mixture, $j = 1 \dots J$.

The main computation algorithm in KYBL-7, leading to consistent balances, is called methods of the results coordination (MRC; Adamczewski 2010). The second algorithm, which is a supporting algorithm mainly used for calculating the starting point for MRC, is based on the Cholesky's method to solve overdetermined systems of equations (MCH).

Method of Results Coordination (MRC)

In practice, the composition of a mine water mixture and the various potential mine water sources are measured values ($M_1 \dots M_I, C_{1,1} \dots C_{I,J}$). These values are often averaged from a set of different measurements at each site. As a result, any mathematical description should take into consideration that the reported mean mine water composition might be error-prone (e.g. measurement, estimation, averaging). This assumption, that the values of M_i and $C_{i,j}$ are likely to include errors, leads directly to the conclusion that the calculated proportions q_j will also be error-prone. After considering the errors in determining the values of $C_{i,j}$, M_i and q_j , the system of equations (1_a...1_i) may be expressed as (Krzeszowski 2009):

$$\sum_{j=1}^J (q_j + \delta_j^q) \cdot (C_{1,j} + \delta_{1,j}^C) = M_1 + \delta_1^M \tag{2a}$$

...

$$\sum_{j=1}^J (q_j + \delta_j^q) \cdot (C_{I,j} + \delta_{I,j}^C) = M_I + \delta_I^M \tag{2i}$$

where:

δ_j^q : errors in the determination of the relative contribution of various sources in the water mixture, $j=1 \dots J$

$\delta_{i,j}^C$: errors in the determination of the sources components, $i=1 \dots I, j=1 \dots J$

δ_i^M : errors in the determination of the water mixture composition, $i=1 \dots I$

The system, after some elementary transformations, assumes the following form:

$$F_1 = \sum_{j=1}^J [(C_{1,j} + \delta_{1,j}^C) \cdot (q_j + \delta_j^q)] - (M_1 + \delta_1^M) = 0 \tag{3a}$$

$$F_2 = \sum_{j=1}^J [(C_{2,j} + \delta_{2,j}^C) \cdot (q_j + \delta_j^q)] - (M_2 + \delta_2^M) = 0 \tag{3b}$$

...

$$F_I = \sum_{j=1}^J [(C_{I,j} + \delta_{I,j}^C) \cdot (q_j + \delta_j^q)] - (M_I + \delta_I^M) = 0 \tag{3i}$$

In summary, the optimum solution, using the method of least squares, is reached when the following set of dependencies are fulfilled:

$$\varphi = \sum_{i=1}^I \sum_{j=1}^J \left(\frac{\delta_{i,j}^C}{\mu_{i,j}^C} \right)^2 + \sum_{i=1}^I \left(\frac{\delta_i^M}{\mu_i^M} \right)^2 + \sum_{j=1}^J \left(\frac{\delta_j^q}{\mu_j^q} \right)^2 \rightarrow \min \tag{4}$$

$$F_1 = \sum_{j=1}^J [(C_{1,j} + \delta_{1,j}^C) \cdot (q_j + \delta_j^q)] - (M_1 + \delta_1^M) = 0 \tag{4a}$$

$$F_2 = \sum_{j=1}^J [(C_{2,j} + \delta_{2,j}^C) \cdot (q_j + \delta_j^q)] - (M_2 + \delta_2^M) = 0 \tag{4b}$$

...

$$F_I = \sum_{j=1}^J [(C_{I,j} + \delta_{I,j}^C) \cdot (q_j + \delta_j^q)] - (M_I + \delta_I^M) = 0 \tag{4i}$$

where:

φ the sum of all unadjusted squares related to maximal, acceptable inaccuracies of the methods used for their determination.

$\mu_{i,j}^C, \mu_j^M, \mu_j^q$: denote, respectively, absolute, acceptable inaccuracies of the methods used for the determination of $C_{i,j}, M_i, q_j$ (e.g. single measurements, averaging from multiple measurements, estimations).

$\delta_{i,j}^C, \delta_i^M, \delta_j^q$: the unknown quantities of the system, the calculation of which enables the designation of the best estimate of values $C_{i,j}, M_i$ and q_j , within the framework of the adopted method.

$C_{i,j}, M_i$: measurement values or values averaged from multiple measurements.

q_j, μ_j^q : unknown values.

In many situations, the equations cannot be sufficiently solved. This might be caused by factors such as additional, unrecorded, or ‘unknown sources’ (such as inflows) contributing to the water mixture, chemical or physical reactions, and other reasons discussed later. Therefore, the sum of all unknown sources of water to the overall water mixture can be considered as an ‘additional water source’. As a result, the mass balance equations for the steady state condition are discussed in this paper with corresponding terms referring to the above mentioned additional water sources using the calculated compositions.

A mixing model of the mine water system may be inconsistent due to physical as well as chemical processes. The identification of these processes would require long-term monitoring and geochemical modeling. Hence, it was assumed that unbalanced results, caused by different chemical or physical processes, can numerically be interpreted as an *equivalent*, or ‘additional water source’. Such methodology allows deriving particular components of the mine waters that are sufficiently known to occur in mines. At the same time, it should be highlighted that the results derived from such a methodology must always be interpreted by a hydrogeologist to avoid hydrogeologically unreasonable results.

Mathematically, the computation used for systems with an equivalent additional water source is identical to the systems without an additional source. The only difference is in the number of the sources contributing to the total water mixture. We will define that the number of water sources is $r = J$ for systems without an additional ‘unknown source’ and $r = J+1$ for systems with an additional source. Equation (4) must therefore be adapted accordingly by substituting J with r .

As the minimum of function φ is a relative extreme, the problem may be solved by the Lagrange method of undetermined coefficients, leading to the derivation of the following objective function:

$$\Phi = \sum_{i=1}^I \sum_{j=1}^r \left(\frac{\delta_{i,j}^C}{\mu_{i,j}^C} \right)^2 + \sum_{i=1}^I \left(\frac{\delta_i^M}{\mu_i^M} \right)^2 + \sum_{j=1}^r \left(\frac{\delta_j^q}{\mu_j^q} \right)^2 + \sum_{i=1}^I (k_i \cdot F_i) \rightarrow \min \tag{5}$$

where $k_i (i=1, \dots, I)$ denote Lagrange coefficients (also called correlates).

The construction of the objective function Φ (5) allows replacing the optimization problem with certain conditions (4) with an optimization problem (5) without such conditions.

The conditions for the existence of the extreme (minimum) of the above objective function are set forth by the following equations:

$$\frac{\partial \Phi}{\partial \delta_{i,j}^C} = 0 ; i = 1, 2, \dots, I, j = 1, 2, \dots, r \tag{6}$$

$$\frac{\partial \Phi}{\partial \delta_i^M} = 0 ; i = 1, 2, \dots, I \tag{7}$$

$$\frac{\partial \Phi}{\partial \delta_j^q} = 0 ; j = 1, 2, \dots, r \tag{8}$$

$$\frac{\partial \Phi}{\partial k_i} = 0 ; i = 1, 2, \dots, I \tag{9}$$

Differentiating equations (6) ... (9) results in equations (10a ... 10d), containing a total of $(I \cdot r + 2 \cdot I + r)$ equations:

$I \times r$ equations of the objective function Φ for variables $\delta_{i,j}^C$:

$$\frac{\partial \Phi}{\partial \delta_{i,j}^C} = \frac{2 \cdot \delta_{i,j}^C}{(\mu_{i,j}^C)^2} + k_i \cdot (q_j^0 + \delta_j^q) = 0 \quad i = 1, 2, \dots, I-1, j = 1, 2, \dots, r \tag{10a}$$

I equations of the derivatives of the objective function Φ for variables δ_i^M :

$$\frac{\partial \Phi}{\partial \delta_i^M} = \frac{2 \cdot \delta_i^M}{(\mu_i^M)^2} - k_i = 0 \quad i = 1, 2, \dots, r \tag{10b}$$

r equations of the derivatives of the objective function Φ for variables δ_j^q :

$$\frac{\partial \Phi}{\partial \delta_j^q} = \frac{2 \cdot \delta_j^q}{(\mu_j^q)^2} + \sum_{i=1}^I k_i \cdot (C_{i,j}^0 + \delta_{i,j}^C) = 0 \quad j = 1, 2, \dots, r \tag{10c}$$

and I equations of the derivatives of Φ unknowns which are Lagrange correlates:

$$\frac{\partial \Phi}{\partial k_i} = F_i = 0 \quad i = 1, 2, \dots, I \tag{10d}$$

The number of the equations is equal to the number of the unknowns in the constructed water system model ($I \cdot r$ corrections $\delta_{i,j}^C$, I corrections δ_i^M , I corrections k_i and r corrections δ_j^q) and is solved using the Gauss elimination algorithm. Solving the equations enables the derivation of the unknowns for the balanced water system, based on the method of least squares at the simultaneous fulfillment of the balance equations (3). All the result must be verified, ensuring that the calculated water proportions are not negative or smaller than one (100%). The quality of the solution is better, the more precise the values of adjustments $\delta_{i,j}^C$ and δ_i^M for, respectively, $C_{i,j}$ and M_i describing the balanced water system.

Cholesky method (MCH)

In a classical approach, the Cholesky method (MCH) derives an unambiguous approximate solution of equation (1). Yet, the MCH is only correct from a mathematical point of view and might result in inaccurate or even incorrect solutions from a physical or chemical point of view. In many cases, the result obtained may be described as a “least negative result” (Gille and Clique 1986, Krzeszowski 2009). In addition, the method misconceives that the values describing the system are error-free, whereas in reality measured data contains errors of various kinds.

To adapt the MCH and MRC methods such that they are able to calculate both, the solution composition and the relative proportion of the ‘unknown source’, it is necessary to incorporate a mechanism for estimating the existence probability of this ‘unknown source’. This mechanism must be able to derive the values of $C_{i,j}$ and M_i as well as the resulting error in the calculation of q_j . We therefore expanded the classical Cholesky method with a simple stochastic approach.

For the calculations assuming the absence of an ‘unknown water source’ contributing to the water mixture we assumed that the MCH consists of a given number of calculation cycles defined by the operator. Each cycle draws on other, random values of $C'_{i,j}$, describing the composition of the water sources. Those $C'_{i,j}$ values are randomly selected from the vicinity of $C_{i,j}$ values, based on ranges defined manually at computation start-up. Their range should be selected such that they provide a good approximation of the single $C_{i,j}$ measurements or designated values.

Mathematically, the selection of $C'_{i,j}$ may be described with the following equation:

$$C_{i,j} \cdot G_{C_i}^D \leq C'_{i,j} \leq C_{i,j} \cdot G_{C_i}^G \quad I = 1, 2, \dots, I, j = 1, 2, \dots, r \quad (11)$$

where:

$C_{i,j}$: content of the i -th component for the j -th source, measured or calculated as the mean value from many measurements

$C'_{i,j}$: randomly changed value of the content of the i -th component for the j -th source,

$G_{C_i}^D$: coefficient of maximal, acceptable deviation “towards zero” for the i -th content of the component (the same for all streams), arbitrarily set by the software operator, $0 < G_{C_i}^D < 1$,

$G_{C_i}^G$: coefficient of the maximal acceptable deviation “from the value of one” for the i -th content of the component (the same for all streams), arbitrarily set by the software operator, $G_{C_i}^G > 1$,

At each computation cycle, the software derives new values of $C'_{i,j}$ from an embedded semi-random number generator (Delphi 2005 built-in linear congruential random number generator). The above-described mechanism of the selection of $C'_{i,j}$ is justified, if it is accepted that $C_{i,j}$ values may be charged with errors resulting from the methodology of their determination. Each single solution of a given computation cycle results in a series of r numbers ($q_1, q_2 \dots q_r$) representing the proportions of the sources in the water mixture. They are computed on the grounds of the matrix analysis by solving I linear equations with r unknowns. Single solutions during the computation are verified on the basis of the following three accuracy criteria (Krzyszowski 2009):

Criterion of the accuracy of the water source proportion values in the water mixture. No water source proportion q_i contributing to the water mixture shall exceed 1 (100%) and no q_i must be negative.

$$0 \leq q_j \leq 1 \quad j = 1, 2, \dots, r \quad (13)$$

Criterion of the sum of the proportions of the inflow water sources. The sum of the calculated proportions of the sources contributing to the water mixture must be within a given range around 1 (100%), where the range is defined at program start up.

$$\sum_{j=1}^r q_j \cong 1 \quad (14)$$

Criterion of the accuracy of the water mixture composition. Even if the above criteria are met, the solution obtained by the MCH might be chemically or physically incorrect. Hence, we assume that the result is correct within a given error range defined at program start up:

$$M_i^{MCH} \cong M_i \quad i = 1, 2, \dots, I \quad (15)$$

where:

M_i^{MCH} : content of the i -th component in the water mixture calculated on the grounds of the values of the proportions of particular water sources by means of the MCH,

M_i : content of the i -th component in the water mixture (measured or the calculated mean value from measurements).

The solutions complying with all of the three above discussed accuracy criteria are regarded as correct. Solutions that meet only the first two criteria are considered supporting, partial solutions. At the end, the final solution is calculated by averaging all r proportions $q_1, q_2 \dots q_r$ of particular water sources in the water mixture of all the simulation runs for one

case. If no single correct solution was derived in the computation process, the end solution is calculated analogically but with the use of the supporting partial solutions. Finally, the end result's uncertainty is the standard deviation of all the proportions q used in the resulting water mixture.

Results and Discussion

Results of the KYBL modelling

Mine waters in the Sokolov Coal Basin generally origin from the mixing of hydrochemically different source waters. The following source waters were defined for the Jiří Mine:

1. Antonín Seam waters (ANT),
2. Sokolov Formation waters (SPA),
3. Cypris Formation waters (CS),
4. Mineral waters from the underlying rocks (Carlsbad type waters KV),
5. Atmospheric rainfall waters (AS).
6. 'Unknown source' (optional)

Multivariate cluster analyses (Ward clustering strategy) was used to identify the hydrogeochemical composition of the source waters. The dendrogram in Fig. 4 shows the hierarchical cluster analyses results calculated separately for the water samples from deep boreholes (OV). Water samples represent Sokolov Formation water (SPA) and Carlsbad type waters (KV). Groundwater samples from the Old Sedlec and Josef Seam formations were included in the clustering as well. However, those two types are not considered a source of the mine water mixture in the mine water sump. The cluster analysis was also used to identify outliers. After removing them from the dataset, the clustering was repeated. The original set of variables (water samples composition) was transformed to a new set of uncorrelated variables using principal component analyses (PCA). This method is generally used for classification, simplification of the data, and finding the most important variables in a data set (Krzanowski 1988). Using standardization of data, two principal components account for 78% of the variance in our dataset. Table 1 presents the results of PCA for two principal components. However, hierarchical cluster analyses of data from PCA without reducing dimensionality resulted in a better visualization than a scatter plot of the two principal components (Fig. 5).

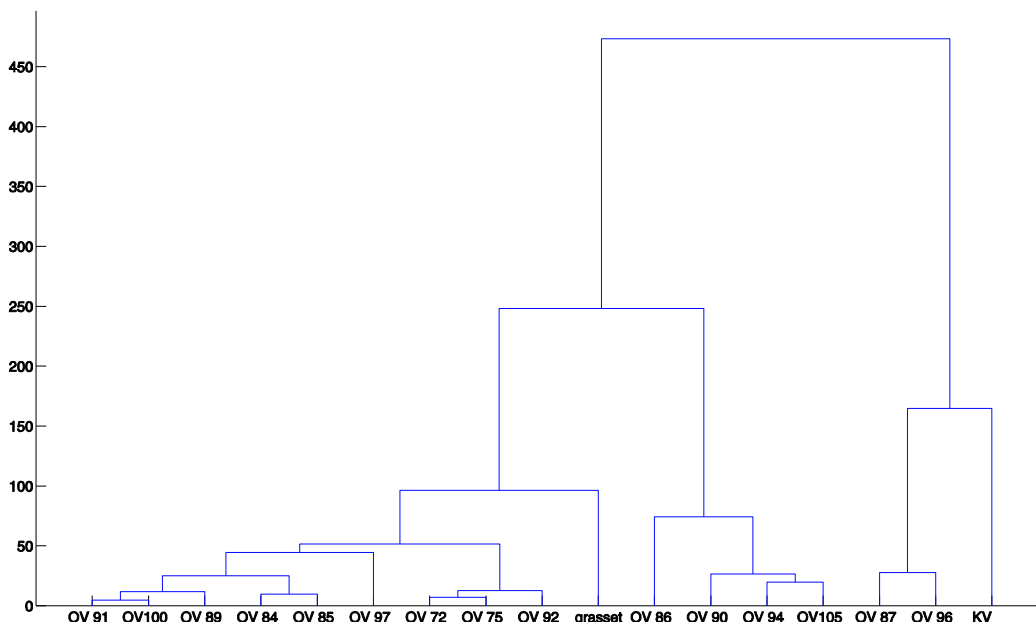


Fig.4 Example of a multivariate cluster analyses for water samples from deep boreholes OV. Borehole number on x axes, distance is unit less number reflecting remoteness of samples. Clusters represent waters from Sokolov Formation and mineral water from underlying rocks. Water sample from Karlovy Vary spa mineral water is included (signed KV) as well as water from Grasset fault inrush

Tab. 1 Output data from PCA – table of components weights

Parameter (mg/L)	Component 1	Component 2
TDS	0.3902	-0.0018
Na ⁺	0.3830	-0.0864
K ⁺	0.3219	0.0839
Ca ²⁺	0.3639	0.0535
Mg ²⁺	0.1772	0.6480
Fe ²⁺	0.1678	-0.2571
NH ₄ ⁺	-0.1026	0.6725
Cl ⁻	0.3519	-0.1254
SO ₄ ²⁻	0.3524	0.1552
HCO ₃ ⁻	0.3833	-0.0677

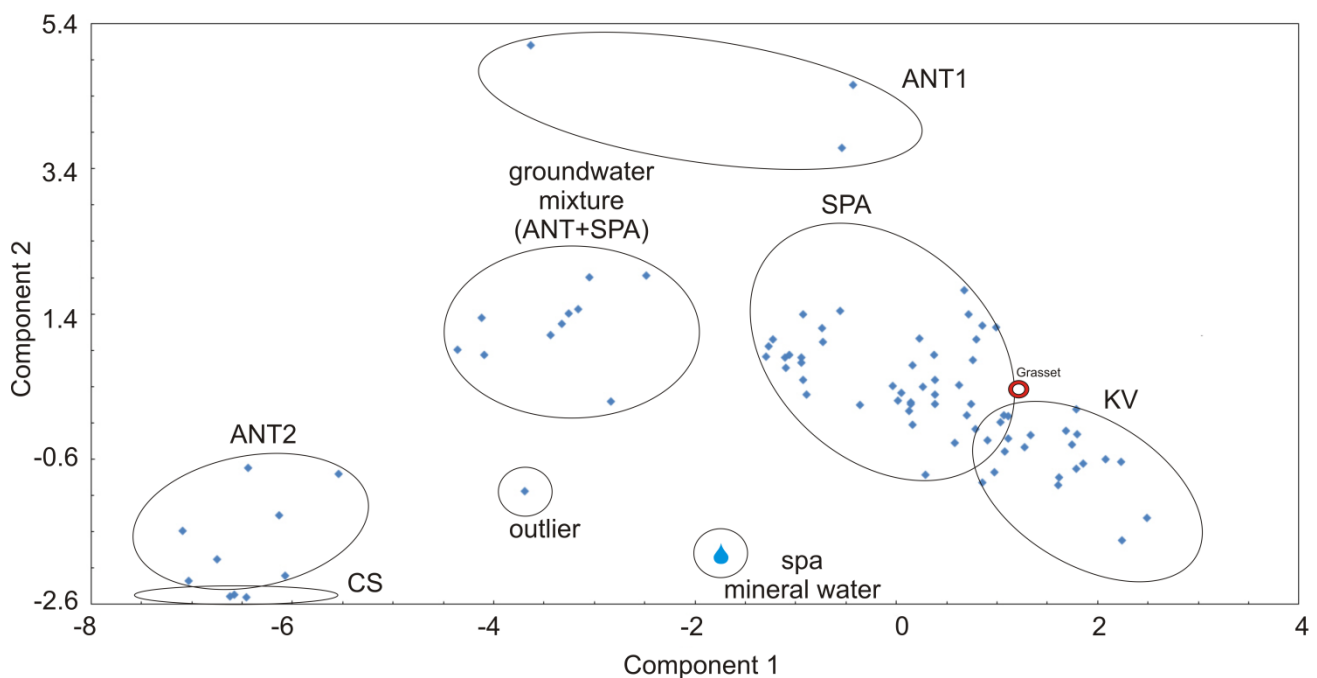


Fig. 5 Scatter plot of principal components. Groundwater sources divided into subgroups depending on the PCA and multivariate analyses

Based on the clustering results, averaged hydrogeochemical compositions of the source waters were calculated. Although several variants of the source water composition were taken into account, we present only one variant in this paper. Since we had different samples and chemical compositions representing the groups of source water, we used generally 10% uncertainty for the mean water composition for each group.

The relationship between the sources and the final mine water mixture is given by equation (1). Inputs for determining the water proportions in the mixture were specified for 10 parameters (Table 2) whereupon the associated ranges of acceptable parameter values reflect data uncertainties due to measurements error as well as parameter variability.

Tab. 2 Example of parameter mean values for the different water sources used and an example range of uncertainties (10%) used for the calculation (in mg/L); ANT: Antonín Seam waters, SPA: Sokolov Formation waters, CS: Cypris Formation waters, KV: Mineral waters from the underlying rocks (Carlsbad type waters), AS: Atmospheric rainfall waters.

Parameter	ANT	SPA	CS	KV	AS	Mixture
TDS	6131±613.1	2274±227.4	940±94.0	9621±962.1	17±1.7	2618±261.8
Na ⁺	1297±129.7	550±55.0	200±20.0	2283±228.3	0.5±0.0	455±45.5
K ⁺	38.6±3.9	36.8±3.7	9.0±0.9	80.6±8.1	1.7±0.2	26.7±2.7
Ca ²⁺	153.3±15.3	65.1±6.5	39.7±4.0	456.9±45.7	0.9±0.1	177.0±17.7
Mg ²⁺	222.7±22.3	21.3±2.1	15.1±1.5	109.0±10.9	0.8±0.1	68.5±6.9
Fe ²⁺	0.5±0.1	8.7±0.9	0.7±0.1	5.1±0.5	0.04±0.1	2.3±0.2
NH ₄ ⁺	1.00±0.1	2.80±0.3	0.20±0.1	1.60±0.2	0.90±0.1	1.37±0.1
Cl ⁻	15.9±1.6	114.5±11.5	7.3±0.7	1089.0±108.9	1.5±0.1	114.0±11.4
SO ₄ ²⁻	3277±327.7	583±58.3	249±24.9	2769±276.9	4.6±0.5	1370±137.0
HCO ₃ ⁻	1012±101.2	920±92.0	400±40.0	2779±277.9	6.3±0.6	381±38.1

The research has been undertaken to quantify the proportions of the sources ANT thru AS in the mine water samples taken from the Jiří Mine dewatering sump. Both methods described in the previous chapter were applied for our analyses.

Technically, the MCH method utilizes a semi-random number generator to generate input data for calculations within the ranges given in Table 2. We set the initial boundary conditions for the computations with the KYBL-7 software as follows: number of simulation cycles 250,000 and 500,000 (the latter only when a relatively small number of positive results were obtained); boundary condition for the source percentage in the mixture between 0.95 and 1.05; boundary condition for the mixture composition between 0.925 and 1.075; number of fitting parameters: 10 (Na⁺, K⁺, Ca²⁺, Mg²⁺, Cl⁻, SO₄²⁻, HCO₃⁻, Fe²⁺, NH₄⁺ and TDS); and number of known sources in the mixture 5. Furthermore, the potential presence of an ‘unknown source’ in the mine water was tested. Depending on the input options, the computation time ranged between hours and tens of hours. In total, we conducted 12 different computations with varying input parameters including and excluding a potential ‘unknown source’.

For all positive solutions of the computation that met the criteria given by equations 13 – 15, we determined average deviations of the source proportions. Results of those simulations are the arithmetic averages of the positive simulations and the dispersal values of the individual solutions. Based on those resulting data, the final proportions of the sources for the mine water were calculated (Table 3) including the results’ dispersions. In the case of scenarios without an unknown source, the solutions have not met all criteria (equations 13 – 15), therefore we proceeded with a scenario including an unknown source.

Tab. 3 The calculation results of proportions of mine water sources in the mine water mixture in % (achieved by the MCH method)

Mine water source	ANT	SPA	CS	KV	AS	‘Unknown source’	Results quality
With “unknown source“	16.3	5.0	12.7	3.2	61.4	1.3	High
	± 2.4	± 3.3	±9.2	± 1.5	± 7.6	± 0.01	

The quality of results is a measure to describe how good the simulations comply with the accuracy criteria described in the text

There are several hypotheses that might explain the ‘unknown source’: (a) a natural, so far unknown source of water, (b) precipitates or secondary minerals dissolved by the mine water, (c) an imbalance in the mixture, caused by the secondary minerals precipitation due to contact of the mine water with the atmosphere (precipitates), (d) evaporation of the mixture in the sump or (e) numerical dispersion of the solver.

In principle, the MCH method cannot give a full balance for the mixture. Both, input data and output results are given in the form of intervals of values. An example of the variation in the proportion of the results for the ANT source in the mixture is presented in Fig. 6. Considering the common uncertainties in hydrogeological problems related to mine water, our stochastic approach in KYBL can be seen as an advantage over current methods. As described above, KYBL-7 offers an MRC method which provides full mass balance results of the mixture including a calculation of the ‘unknown source’ composition. It requires an initial estimate of the proportions of the mine water’s sources using the results of the MCH method which is supposed to be a good approximation. As a result, the MRC method produces proportions of water sources in the mine water mixture (e.g. in the mine sump) as well as corrections of the input data within the allowed

interval (Table 4). Finally, KYBL calculates the corrected chemical composition with very small changes much below 1% of the initial values which are presented in Table 5.

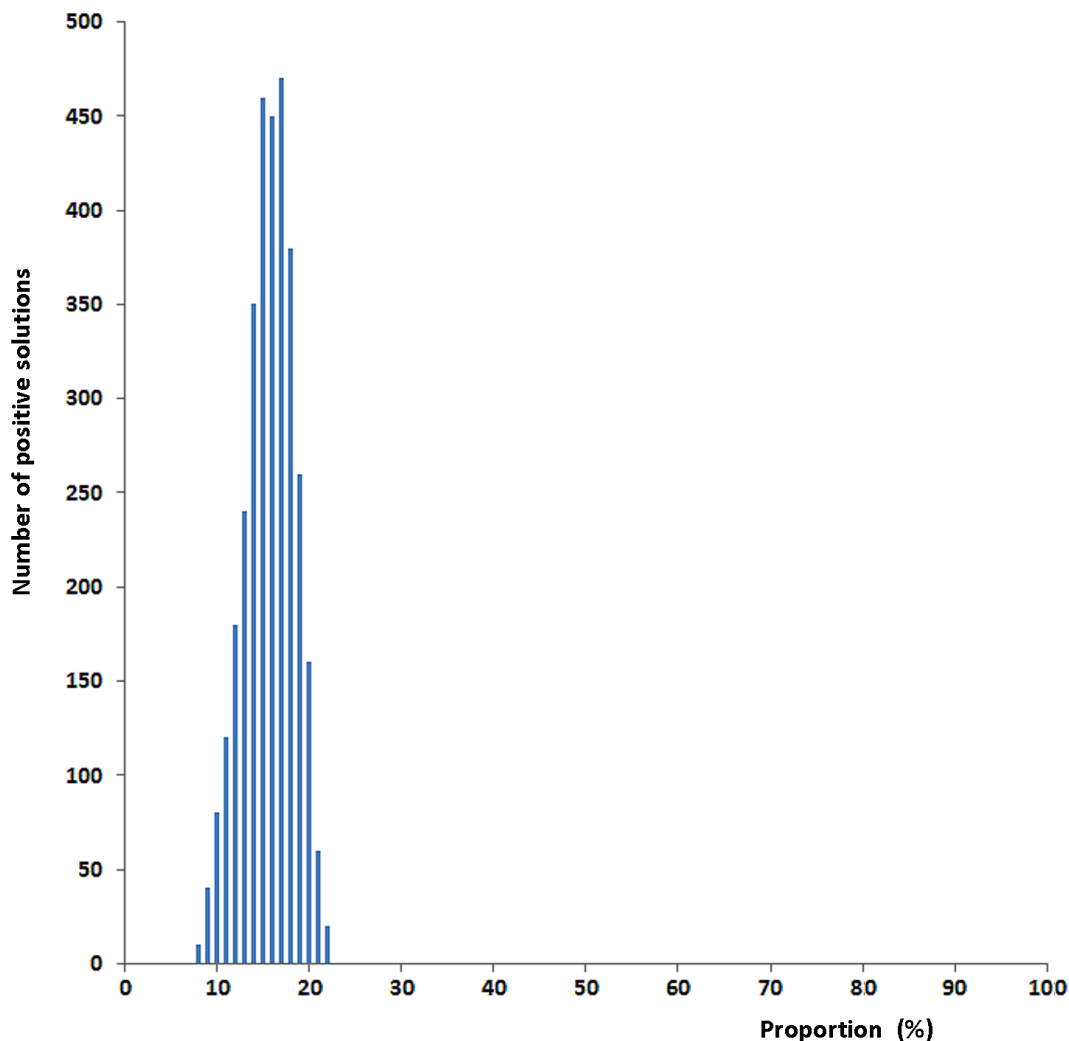


Fig. 6 Dispersion of the results (MCH method). Proportion of ANT source in the mixture on x axis. Number of positive solutions on y axis

Tab. 4 Calculated corrections of input data values – MRC method (data in mg/L)

Parameter	ANT	SPA	CS	KV	AS	Mixture
TDS	-7.0199	-0.2988	-0.1285	-3.3906	-0.0002	7.8508
Na ⁺	3.9191	0.2180	0.0722	2.3817	0.0000	-2.9594
K ⁺	0.0432	0.0122	0.0018	0.0370	0.0003	-0.1269
Ca ²⁺	-0.3693	-0.0206	-0.0193	-0.6433	0.0000	3.0190
Mg ²⁺	1.5693	0.0044	0.0056	0.0737	0.0001	-0.9106
Fe ²⁺	0.0000	-0.0005	0.0000	-0.0001	0.0000	0.0007
NH ₄ ⁺	0.0002	0.0012	0.0000	0.0004	0.0001	-0.0219
Cl ⁻	-0.0019	-0.0300	-0.0003	-1.7186	-0.0001	0.5889
SO ₄ ²⁻	-9.4800	-0.0929	-0.0426	-1.3273	-0.0001	10.1601
HCO ₃ ⁻	6.3601	1.6278	0.7740	9.4053	0.0009	-5.5299

Tab. 5 Final results after corrections of data values (rounded), parameter values in mg/L

Source	ANT	SPA	CS	KV	AS	Unknown source	Mixture
Proportion (%)	16.3	5.04	12.69	3.19	61.43	1.35	
TDS	6123.78	2273.50	939.87	9617.51	17.26	79554.81	2625.85
Na ⁺	1300.62	550.02	199.57	2284.88	0.47	8413.93	452.04
K ⁺	38.64	36.81	9.00	80.64	1.72	1008.57	26.57
Ca ²⁺	152.93	65.08	39.68	456.26	0.90	9729.43	180.02
Mg ²⁺	224.27	21.30	15.11	109.07	0.76	1781.03	67.59
Fe ²⁺	0.50	8.70	0.70	5.10	0.04	108.24	2.26
NH ₄ ⁺	1.00	2.80	0.20	1.60	0.90	30.64	1.35
Cl ⁻	15.90	114.47	7.30	1087.28	1.45	5152.40	114.59
SO ₄ ²⁻	3267.82	583.01	248.96	2767.67	4.58	51393.57	1380.16
HCO ₃ ⁻	1018.26	921.93	400.77	2787.91	6.25	1437.25	375.47

In any case, ten selected parameters of the ‘unknown source’s’ hypothetical chemical composition (Table 5) exceed the parameters of five real solutions in some cases by two orders of magnitude.

Geochemical modeling with the chemical-thermodynamic code PHREEQC (Parkhurst et al. 1999) proved that the computed imbalance is due to site specific geochemical processes and the ‘unknown source’ – in fact – does not represent an additional water source. The modeling also proved that gypsum and/or anhydrite were decisive phases in the sampled waters with saturation indices of gypsum ranging from 1.43 to 2.09, eliminating any long-term stability of such solutions. As such, the solutions would rather represent a gypsum crystal suspension, or gypsum itself, while the gypsum sediment would be settled at the bottom of the reservoir. In the case of the carbonate phases, the saturation indices of calcite, or aragonite and dolomite, are critical and their strong oversaturation is an indication for the neutral or alkaline reaction of the solutions. It can be assumed that the unknown source represents the mass balance mixture of two types of solution: the first one deriving from pyrite weathering products (high content of sulphates and Fe, pH below 4) and the second one from the dissolution of mineral water evaporates (high hydrogen carbonates). Both, secondary minerals and minerals from mineral water evaporation can be found within the pit and are dissolved during precipitation, hence contributing to the final composition of the mine water mixture.

Comparison with NETPATH

In order to verify the mixing results of KYBL we ran a mixing model using NETPATH XL (Plummer et al. 1994). As described above, NETPATH can identify the ratios of up to five different water sources contributing to a final water composition. We used the mean composition for the source waters based on Table 2 and assumed that here is no additional source water involved. Because NETPATH needs an initial pH, temperature and redox value for the calculation, we set the temperature to 20 °C, the pH to 7 and the redox potential was 300 mV in the model. Based on the species distribution in the 5 source waters we selected 18 phases for the model (Aragonite, Brucite, Calcite, CO₂ gas, Dolomite, Fe²⁺-Na, Gypsum, Hematite, Magnesite, Mg₂CO₃, Mg/Na ex, Mirabilite, Na₂SO₄, NaCl, NaHCO₃, Pyrite, Siderite, Sylvite) and used 8 of the analyzed parameters (C, Ca, Cl, Na, S, Mg, Fe, K). This input data resulted in 31824 potential models and 710 valid models were found. Out of those there were only 25 models which included all the 5 wells as source waters but only 2 different source water ratios were calculated.

The first potential model consists of 91 % rain water and the 4 other sources contribute relatively evenly distributed to the remaining 9 % (Table 6). A high evaporation factor of 5.332 in this model is the reason why the final composition of the mixed mine water is closely met. The second potential model is composed of 7.1% ANT, 17.8% SPA, 45.6% CS, 7.5% KV, and 21.9% AS. As can be seen in table 7, using this source water ratio in a mixing calculation with PHREEQC results in a very similar mixture water composition as listed in Table 2. No evaporation was calculated by NETPATH for this second mixing proportion. Except for the carbon species and for Ca as well as the sulfur species, the results obtained by using NETPATH and PHREEQC are very similar to the real composition of the mixed mine water. This is due to the fact that the proportion of the highly mineralized Carlsbad type waters in model NETPATH2 is higher than the other two and therefore results in higher concentrations in the carbon and sulfur species. In a future model it would be necessary to modify the input parameters for NETPATH within the ranges given in table 2 to obtain better mixing ratios.

Tab. 6 Modeling results of NETPATH using the source water composition of table 2.

Model Number	ANT	SPA	CS	KV	AS	'Unknown source'
NETPATH 1	2.2	3.4	2.4	1.4	90.6	–
NETPATH 2	7.1	17.8	45.6	7.5	21.9	–
KYBL	16.3	5.0	12.7	3.2	61.4	1.3

Tab. 7 Results of a mixing calculation with PHREEQC using the source water ratio of model NETPATH 2. Results in mmol/L.

Element	PHREEQC	Mixture
C	14.770	7.436
Ca	1.885	4.428
Cl	3.041	3.224
Fe	0.041	0.041
K	0.510	0.685
Mg	1.442	2.825
N	0.070	0.098
Na	19.810	19.843
S	10.870	14.299

Comparing the NETPATH result with the KYBL result makes clear that the Carlsbad type waters contribute only at a small portion to the final composition of the mine water in the open pit. Evaporating rain water and the Cypris formation water are the main contributors to the final mine water composition in the Jiří and Družba pits.

Conclusions

The paper aimed at presenting the newly developed computer code KYBL and its application exemplified by a case study from the Sokolov Coal Basin. This code represents the inverse solution of the mixing equation accounting also for the variability of the initial data set (uncertainty). It enables to calculate proportions of up to 10 sources (defined by 4–12 hydrochemical parameters) in mine water mixtures without reducing the multiparametric information. KYBL could be used as a first step in mixing and mass transfer calculations to complement calculations with a chemical-thermodynamic code such as PHREEQC or a mixing calculation with NETPATH. As has been shown, those codes can then use the calculated mixing proportions for the source waters based on KYBL.

KYBL computational methodology is generally based on the assumption of steady state (both hydrodynamic and geochemical) of mine water sources. But similarly to numerical groundwater modeling techniques the time periods can be designed corresponding to changes of mine water regime. Changes of hydrodynamic and geochemical state (mine water sources number and their quality) can be introduced into calculation for designed time periods. This approach of time discretization makes analyses more sophisticated and complex. It fully corresponds to numerical modeling of groundwater flow and solute transport where sources and sinks in transient simulation are assumed to be constant within designed time period (time discretization).

Our methodology of quantifying proportions of mine water sources in a water mixture based on hydrochemical data of different sources has already been applied successfully at several other mines in the Czech Republic and Poland. In the case of underground mines, no relevant imbalance of the results was found, whereas in open pit mines geochemical reactions typically seem to introduce imbalances in the mixing equation. While solving the sets of overdetermined mixing equations, KYBL elides geochemical reactions occurring during the mixing of individual water sources or during the water-atmosphere-contact. This distinguishes the code from chemical-thermodynamic packages such as NETPATH, PHREEQC, or Geochemist Workbench. KYBL is a mere mathematical and statistical solver of the mixing equation, approximating the proportions of the individual sources to give the closest mine water composition. This process and a simple use were incubated in the program development to meet the needs of mining hydrogeologists and engineers. It might take into account the variability of the sources, natural and technological conditions in the open pit operation, anthropogenic loads, and errors in sampling and analyses.

It is obvious from the results that the 'unknown source' can be seen as a form of geochemical disequilibrium or numerical dispersion. On our case study, geochemical reactions were confirmed by means of geochemical modeling with

PHREEQC as well as the mixing model with NETPATH showing a relatively high evaporation factor for one model, and are verified by the field surveys. The calculated KYBL results of our case study showed that the relative proportion of the Carlsbad type waters in the mine water mixture of the Jiří and Družba Mines is relatively low at $3 \pm 1.5\%$, a result which was also proven by a mixing calculation with NETPATH.

Structural and geological analysis as well as hydrogeological studies have shown that the prospecting and mining activities in the Sokolov Coal Basin have had no impact on the flow paths of the Carlsbad hot springs. The two hydrogeological relevant structures, the Carlsbad hydrothermal structure and the Sokolov hydrothermal structure, are virtually independent from each other. A possible connection between both structures is indicated by juvenile CO_2 existing in both the Carlsbad hot springs and the Sokolov Coal Basin. Due to this CO_2 , the monitoring measures and the calculation described in this paper were undertaken. They shall ensure that the thermal springs in the world famous Carlsbad spa are long-term protected from potential impacts by the coal mining operations in the Sokolov Coal Basin.

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