Methodology of Quantitative Assessment of Mine Water Inflows

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

Keywords Mine water sources proportions, open-pit coal mining, mixing equation, geochemical modeling, water balance.

Introduction

Chemical compositions of mine waters are a result of several mechanisms depending on the type of mining operation and the geological setting (*e.g.* surface, underground mining, soft rock, hard rock). Knowledge of the proportional inflow rates from the individual aquifers may facilitate the prediction of chemical trends of the mine water mixtures. In numerical models, the individual inflows from different aquifer systems contributing to the overall chemistry result indirectly from the calculation results. They are based on the calibration targets of hydraulic heads, the estimated hydraulic conductivities of the aquifers, and the total dewatering rate (Rapantova *et al.* 2007).

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 with particular methods used in the mining environment (*e.g.* Brassington 2006; Wolkersdorfer 2008). 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).

This paper will present an alternative indirect method of calculating the proportions of mine water inflows into a mine water sump by using a case study from the Sokolov Coal Basin, Czech Republic. 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 (Krzeszowski *et al.* 2005; the Czech word 'kýbl', derived from the German word 'Kübel', means 'bucket', used in mine shaft construction).

Numerical codes for mixing calculations

Basically, the philosophy of calculating the proportions of water sources in a mine water mixture used by KYBL-7 is very similar to that of the code M3 (Multivariate Mixing and Mass balance calculation; Laaksoharju *et al.* 1999, Laaksoharju *et al.* 2008). Both codes utilize hydrochemical data for calculating 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 for further modeling. M3, as declared by the authors, should only be used if two principal components of the data set sum up to more than 60 % of the variability of the information in the data set. According to Gómez *et al.* (2008), mass balance calculations in M3 are much more sensitive to non-conservative compositional variables and their recommendation 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 waters is NETPATH (Plummer *et al.* 1994). This inverse geochemical modeling code takes into consideration two to five 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 using chemical thermodynamic principles. 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 might result in large sets of mixing proportions and mineral mass transfers. Consequently, the application of this methodology might become very difficult and tedious when applied to large groundwater datasets (Gómez *et al.* 2008).

Methods

In order to protect the Carlsbad hot springs, it is necessary to quantify and determine the proportion of the Carlsbad type waters in the drainage water of the Jiří and Družba open pit mines in the Sokolov Coal Basin (Czech Republic). Those calculations, where proportions of various waters contributing to a water sample have to be calculated, are an essential problem in applied hydrogeology. 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.

For the source identification of the mine water in the Jiří and Družba open pit mines, chemical analyses of groundwater taken from boreholes between 2004 and 2006 were used. By means of multivariate cluster analyses the hydrogeochemical data of the groundwater from the dewatering boreholes was characterized. Cluster analysis was conducted with the Ward clustering method of MATLAB (Manly 1994), which computed a dendrogram including similarity/dissimilarity values for samples and statistical data characterizing the individual clusters. A total of 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+}. In order to transform the original set of variables (the chemical composition of the water samples) to a new set of uncorrelated variables we applied principle cluster analyses (PCA; Jolliffe 1986), which is generally applied for classification, simplification of data and finding the most important variables in a data set (Krzanowski 1988). The transformed water composition was obtained by using the centers of the clusters. To verify that the transformed composition is chemically and statistically similar to the original data, we run hierarchical cluster analyses on both the original and the transformed data matrix identifying no statistically significant difference.

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 (Krzeszowski 2005, 2009, Krzeszowski *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. 1 shows the conceptual model applied by means of KYBL-7.

The whole set of mathematical equations that describe the fractions of the different source waters are based on the following equations:

$$\begin{aligned} \sum_{j=1}^{J} q_j \cdot C_{1,j} &= M_1 \\ &\vdots \\ \sum_{j=1}^{J} q_j \cdot C_{1,j} &= M_1 \end{aligned} \qquad (1)$$

where:

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

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

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

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). Both algorithms are described in detail in Rapantová *et al.* 2012.

Results and Discussion

Mine waters in the Sokolov Coal Basin result from the mixing of hydrochemically different water sources. For the Jiří Mine, the following six potential water sources were defined: Antonín Seam waters (ANT), Sokolov Formation waters (SPA), Cypris Formation waters (CS), Mineral waters from the underlying rocks (Carlsbad type waters KV), Atmospheric rainfall waters (AS), and a potentially unidentified source (PUS; optional).

Based on the clustering results with two principal components accounting for 78 % of the variance in the dataset, averaged hydrogeochemical compositions of the source waters were calculated using the. Although twelve averaged alternatives of the source water composition were applied in the study, we present only one of those in this paper. To represent the chemical variations of the water chemistry within each group as well as measurement errors, we applied a 10 % uncertainty resulting from potential analytical or sampling errors to the mean water compositions (Table 1).

Technically, the MCH method utilizes a semi-random number generator for the generation of input data within the ranges given in Table 1. We defined the initial boundary conditions for the computations in KYBL-7 as follows: number of simulation cycles 250,000 or 500,000 (the latter only when a relatively small number of positive results were obtained); boundary condition for the proportion of the source water in the pit water between 0.95 and

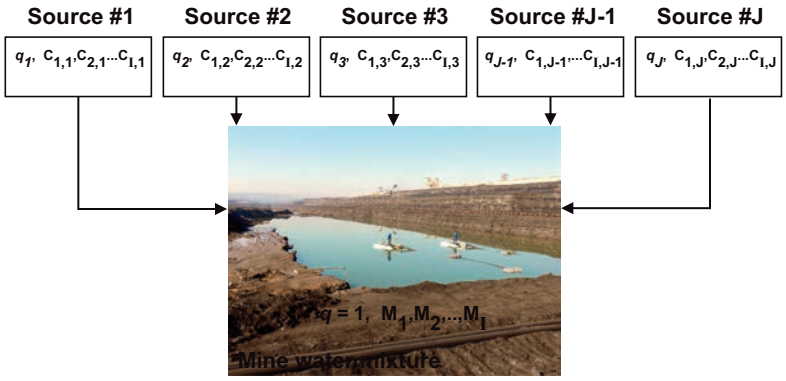

Fig. 1 *Diagram of the water mixture for J mine water sources with known compositions ($c_{i,j}$) and unknown proportions (q_j) in water mixtures with known compositions (q. M_i). Unknown variables, constituting the unknown quantities of the system are italised.*

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

Table 1 *Example of a parameter set with mean values for the different water sources. A 10 % uncertainty for all samples was assumed (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.*

1.05; boundary condition for the mixture composition between 0.925 and 1.075; number of fitting parameters: 10 (Na^+, K^+, Ca^{2+}, Mg^{2+}, Cl^-, SO_4^{2-}, HCO_3^-, Fe^{2+}, $NH4^+$, and TDS); and number of known sources in the mixture 5. Furthermore, the hypothesis of a potentially unidentified source contributing to the pit water chemistry was tested. Depending on the input options, the computation time ranged between hours and tens of hours. In total, we conducted twelve different computations with varying input parameters including and excluding the potential unidentified source.

For all valid computation solutions, we determined average deviations of the source proportions. Results of those simulations are the arithmetic averages of the valid 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 2) including the results' dispersions. None of the scenarios excluding the potentially unidentified source met al. l predefined criteria; therefore we preceded the calculations with a scenario including the potentially unidentified source.

Several hypotheses could explain the existence of the potentially unidentified 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 mine water mixture. Therefore, both, the input data and output results are provided as intervals of values. Consid-

Mine water source	ANT	SPA	CS	KV	AS	PUS	Results quality
With potentially unidentified source	16.3 ± 2.4	5.0 ± 3.3	12.7 ± 9.2	3.2 ± 1.5	61.4 ± 7.6	1.3 ± 0.01	High

Table 2 *Calculation results of proportions of mine water sources in the mine water mixture in % (achieved by the MCH method); PUS: potentially unidentified source. No geochemically viable results were obtained for models without the PUS. The results quality is a measure to describe how good the simulations comply with the accuracy criteria.*

ering the common uncertainties in hydrogeological problems related to mine water, KYBL's stochastic approach can be considered an advantage over current methods. As described above, KYBL-7 employs an MRC method which provides full mass balance results of the water mixture including a calculation of the potentially unidentified 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. Finally, KYBL calculates the amended chemical composition of the averaged sources with very small changes much below 1 % of the initial values (Table 3).

As can be seen from table 3, the ten calculated physico-chemical parameters of the PUS exceed the six associated chemical parameters of the real sources of up to two orders of magnitude. This was an indication for the PUS to be not an additional, real water source. To identify the meaning of the PUS for the overall composition of the pit water, we conducted a geochemical modeling with the chemical-thermodynamic code PHREEQC (Parkhurst and Appelo 2013). This modeling proved that the PUS is due to site specific geochemical processes and – in fact – does not represent an additional water source. Saturation indices (SI) of gypsum were relatively high in all those calculations, ranging from 1.43 to 2.09, eliminating in fact 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 phases of carbonates, the saturation indices of calcite, or aragonite and dolomite, are vital. In case of carbonates, any strong oversaturation of the solutions will only appear subject to a neutral or alkaline reaction of the solutions. It can be assumed that the unknown source represents the mass balance mixture of two types of solutions. The first one comes from dissolution of pyrite weathering products (high content of sulphate and Fe, pH below 4), the second one form dissolution of mineral water evaporates (high hydrogen carbonates). Both, secondary minerals and minerals from mineral water evaporation are exposed in the pit and dissolve during precipitation, hence contributing to the final composition of the mine water mixture.

Conclusions

The paper aimed at presenting the newly developed computer code KYBL-7, exemplified by a case study from the Sokolov Coal Basin,

Source	ANT	SPA	CS	KV	AS	PUS	Mixture
Proportion (%)	16.3	5.04	12.69	3.19	61.43	1.35	–
TDS	6123.8	2273.5	939.9	9617.5	17.3	79554.8	2625.9
Na^+	1300.6	550.0	199.6	2284.9	0.5	8414.0	452.0
K^+	38.6	36.8	9.0	80.6	1.7	1008.6	26.6
Ca^{2+}	152.9	65.1	39.7	456.3	0.9	9729.4	180.0
Mg^{2+}	224.3	21.3	15.1	109.1	0.8	1781.0	67.6
Fe^{2+}	0.5	8.7	0.7	5.1	0.0	108.2	2.3
NH_4^+	1.0	2.8	0.2	1.6	0.9	30.6	1.4
Cl^-	15.9	114.5	7.3	1087.3	1.5	5152.4	114.6
SO_4^{2-}	3267.8	583.0	249.0	2767.7	4.6	51393.6	1380.2
HCO_3^-	1018.3	922.0	400.8	2787.9	6.3	1437.3	375.5

Table 3 *Final results after computed amendments of input data (rounded), parameters in mg/L; PUS: potentially unidentified source*

Czech Republic. This code represents an inverse solution of the mixing equation accounting also for the variability of the initial data set (uncertainty). It encompasses calculating up to ten source proportions (defined by four to twelve hydrochemical parameters) in mine water mixtures without reducing the multiparametric information. KYBL-7 can be used as a first step in mixing and mass transfer calculations to complement chemical-thermodynamic (*e.g.* with PHREEQC) or mixing calculations (*e.g.* with NETPATH). As has been shown, those codes can supplement to the results of KYBL by using its calculated mixing proportions for the source waters.

Our methodology described in this paper has already been applied successfully at several 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 (*e.g.* NETPATH, PHREEQC, Geochemist Workbench). KYBL is purely based on mathematical and statistical procedures to solve the general mixing equation by approximating the proportions of the individual sources to give the closest mine water composition. The guiding idea behind the development of KYBL was to provide a simple usage based on the before described approach in order to meet the applied needs of mining hydrogeologists and engineers. It takes into account the variability of the sources, natural and technological conditions in the open pit operation, anthropogenic loads, and errors in sampling and analyses.

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