Hydrochemical Characteristics Analysis and Water Source Recognition for the Mixed Mine Water: A Case Study of the Jinggezhuang Mining Area

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Abstract

Hydrochemical analysis is one of the most efficient and simple methods to distinguish the source of mine water inrush. However, in reality, its applicability has been restricted hugely due to the mine water inrush source are usually the mixed one. In this study, taking Jinggezhuang mining area as an example, the hydrochemical characteristics of the mixed mine water (the mixture of the ordovician limestone water, k6-coal 12, coal 9-coal 7, coal 5 roof sandstone water and the alluvial loose aquifer at a ratio of 1:9, 2:8, 3:7, 4:6, 5:5, 6:4, 7:3, 8:2 and 9:1, respectively) were firstly investigated by the water quality test; secondly, the mixed reaction mechanism was rapidly obtained using the irreversible reaction simulation model of PHREEQC, and also established a water mixed reaction model applied for Jinggezhuang mining area by the error analysis of hydrochemical compositions of water bursting point and the standard values. The result indicates that the concentrations of main ions in the mixed water all showed an decrease tendency with continuously extend of ordovician limestone water. The variation of Na^+, SO_4^{2-}, HCO^3_- is smoother, K^++N^{a+} decreased from 19.5 mg/L to 12.5mg/L, SO_4^{2-} is reduced from 35.8 mg/L to 17.9 mg/L, and HCO_{3-} shifted from 207.2 mg/L to 159.3 mg/L. In addition, Total Dissolved Solids (TDS) and the mineralization is also gradually decreasing with a large percentage of ordovician limestone water, whereas the total hardness and PH getting bigger. By discriminant analysis of the 4 unknown water points, the recognition precision of the model is up to more than 90% based on the Bayes model, it is expected to provide a scientific basis for the rapid identification of mine water inrush sources.

Keywords: mine; mixed mine groundwater; water inrush sources; water mixed reaction model

Introduction

Coal mine water inrush restricts the safe and efficient production of coal mines, and the economic losses caused by coal mines are also in the first place. It is urgent to find high-precision methods and techniques for identifying the source of water inrush. Scholars have done a lot of research on the identification and prediction of water inrush from different aspects: some studies were performed on identifying the source of water inrush from the perspective of water inrush mechanism. Considering rock mass structure, rock mass strength and mining fragmentation, the study mostly proceeds from the dynamic balance of coal seam roof and floor. The critical equilibrium state of rock mass is taken as the control condition of water inrush from floor of coal seam. This method is used to prevent and identify the source of water inrush by calculating the stress of rock mass before and after mining and some tectonic stresses such as faults. In this respect, the Slesalev formula, the vulnerability index method (Zhang 2008, Wu 2007, Wu 2008, Wu 2009) and the "lower three zones" theory (Ling 2003, Shi 2007), the geomechanical method(Jin 2000, Zhang 2005, Kong 2008), the key strata theory (Du 2008, Wang 2002) have been formed.

There were other studies focusing on identifying water sources by analyzing background values of aquifers. By analyzing the data characteristics of groundwater chemistry, water level and water temperature in different aquifers, the source of water inrush can be distinguished from the hydrochemical and physical information of water inrush (Yang 2003, Chen 2005, Du 2006, Liu 1999, Liu 2001, Li 2008). The most important method is the hydrochemical analysis method, that is, the analysis of water quality types, physical and chemical characteristics of water samples, combined with the hydrogeochemical distribution, migration and transformation of water quality to analyze the source of water inrush. The object of study is divided into conventional hydrochemical characteristics, isotopes and trace elements. Hydrogeochemical exploration technology is fast, timely and economical in recognizing the source of mine water inrush. Therefore, Therefore, the method of recognizing the source of mine water inrush by conventional hydrochemical information has been widely studied and applied.

In recent decades, with the extensive development of computer application in coal mine water inrush, such as probability index method (Wu 2007), multivariate statistical method (Liu 2001), analytic hierarchy process (Dong 2014, Liu 2000), fuzzy mathematics method (Yu 2007, Sun 2007), grey relational degree evaluation method (Li 2008, Zhang 2007, Gao 2007), neural network method (Wei 2004), extension identification method (Zhang 2009), etc. The common characteristic of these methods is that by comparing and sorting the similarity degree of chemical data between inrush water samples and possible water sources, or sorting according to the probability of occurrence, the largest result is the inrush water source.

In terms of multivariate statistics, Li Zhifeng (2008) used Fisher model to discriminate the source of water inrush, Guihe Rong and Chen Luwang (2008) used Bayesian discriminant model to discriminate the source of water inrush. Dong Donglin (2012) used a GIS-based Bayesian network (BN) to assess water-inrush situation. As for the method of fuzzy mathematics, Liu Wentao (2000) and others used the analytic hierarchy Process-Fuzzy evaluation to evaluate the safety of floor water inrush. Sun Yajun et al. (2007) got the background value of aquifer based on GIS, and used clustering analysis and fuzzy comprehensive evaluation to identify the source of water inrush, and achieved good results. In the grey relational degree evaluation method, Li Qikang (2008) and Zhang Honggang (2007) used the grey situation decision-making method to distinguish the source of water inrush. In the aspect of neural network method, Wei Yongqiang (2004) expressed and quantified the factors causing water inrush by using GIS technology, obtained training data by using evidence weight method and analytic hierarchy process, and then predicted floor water inrush by using neural network. They all have been achieved good results.

At present, there are few studies on the hydrochemical characteristics of the mixed water from multi-aquifers, but are relatively rare on the aquifers in North China of Jinggezhuang Mine. Therefore, considering the actual water inrush situation, taking Jinggezhuang Mine as an example, this paper was undertaken to explore hydrochemical characteristics of the mixed water basen on the numerical model in PHREEQC and establish a water mixing reaction model suitable for Jinggezhuang mining area by the Bayes discriminant method. It is expected to provide a reference for the recognition of Water Inrush Source in this mining area in the future.

Methodology

Data acquisition

The hydrochemical characteristics data of aquifers are obtained in Jinggezhuang Mine, including the aquifer where the water samples are located, the pH value and the concentration of cations and anions (Na+, Ca^{2+}, Mg^{2+}, Fe^{2+}, Fe^{3+} Al^{3+}, NH^{+}, Cl^{-} SO_4^{2-}, CO_3^{2-}, HCO^{-}, NO^{3-}, NO^{2-}) in the water. The aquifers in Jinggezhuang Mine are Ordovician limestone aquifer, K6-coal 12 aquifer, coal 9-coal 7 aquifer, coal 5 roof sandstone aquifer and Quaternary loose alluvium. The

Table 1 Primary Hydrochemical Data of Water Samples in Jinggezhuang Aquifers

Aquifer	Ordovician limestone	K6-coal 12	Coal 9-coal 7	Coal 5 roof sandstone	Quaternary loose alluvium
pH	7.84	7.66	8.10	8.30	7.50
Na^{+} (mg/L)	11.64	20.40	36.05	88.74	6.25
Ca^{2+}(mg/L)	46.27	59.78	44.77	34.23	14.97
Mg^{2+}(mg/L)	12.54	23.84	15.61	6.01	30.46
Fe^{2+}(mg/L)	0.00	0.00	0.00	0.00	0.20
Fe^{3+}(mg/L)	0.00	0.00	0.00	0.04	0.06
Al^{3+}(mg/L)	0.00	0.00	0.01	1.69	0.68
NH^{+}(mg/L)	0.00	0.00	0.24	0.00	0.00
Cl^{-}(mg/L)	18.99	10.22	9.81	17.97	7.93
SO_4^{2}(mg/L)	15.71	37.99	10.19	15.00	1.65
HCO^{-}(mg/L)	153.34	213.21	282.63	261.92	47.89
NO^{3-}(mg/L)	30.33	0.00	0.00	0.53	23.01
NO^{2-}(mg/L)	0.00	0.12	0.00	0.00	0.00

hydrochemical characteristics of each aquifer are shown in Table 1.

Water sample mixing simulation based on PHREEQC

PHREEQC is a hydrogeochemical simulation software developed by American Geological Survey (Parkhurst 1999). For multi-solute solutions, PHREEQC uses a series of equations to describe water activity, ionic strength, solubility equilibrium of different phases, charge balance of solution, equilibrium of element composition, mass conservation of adsorbent surface, etc. According to the user's command, PHREEQC will select some of the equations to describe the corresponding chemical reaction process (Mao Xiaomin 2004).

Hybrid simulation function of PHREEQC hydrogeochemical simulation software: Hybrid function can simulate two kinds of water samples mixed in different proportions, and finally get the water sample information in equilibrium state. Forward simulation can calculate the specific content of ions in saturated water samples by mixing equilibrium simulation using the given composition of water samples and ion concentration, and analyze their hydrochemical characteristics.

The water samples from different aquifers in Jinggezhuang Mine were mixed by PHREEQC, and the mixing ratios were 1:9, 2:8, 3:7, 4:6, 5:5, 6:4, 7:3, 8:2 and 9:1, respectively.

Bayes Multi-class Linear Discrimination Principle

Bayesian discriminant analysis uses Bayesian probability rule to discriminate. Its theoretical basis is more supported by statistical theory than Fisher's typical discriminant analysis. Beginning with the multivariate distribution of samples, Bayes makes full use of the information provided by the probability density of multivariate normal distribution to calculate the posterior probability (Wu Guanmao 2008).

For n samples taken from G matrices and each sample contains P variables, each sample can be regarded as a point in P-dimensional space. For an unknown sample, the probability of falling into which subspace is high, that is to say, it belongs to this parent. At the same time, there must be a phenomenon of misclassification, which will cause losses. When the losses of any research individual X= (x1, x2,... xn) caused by other parent is greater than that caused by Ag parent, it is classified as Ag parent. Therefore, Bayes criterion is to minimize the loss of misclassification {R} when the prior probability QG of the parent is given.

If the probability of misclassification of samples originally belonging to parent Ag into Ah is recorded as P {h/g}, when the probability distribution fg(x) of G parent Ag is known, there are:

$$P(h,g) = \int_{Rh} f_g(x)dx$$

The average loss caused by misclassifying a sample originally belonging to the parent Ag to the parent Ah is:

$$W_h = \sum_{g=1,g\neq h}^{G} L(h/g)P(h/g) = \sum_{g=1,g\neq h}^{G} L(h/g)\int_{Rh} f_g(x)dx$$

The average loss of the G-type parent when the prior probability qh of each parent is known is:

$$W_R = \sum_{g=1}^{G} q_h W_h = \sum_{g=1}^{G} q_h \sum_{g=1,g\neq h}^{G} L\{h/g\}P\{h/g\}$$

If the sample originally belonging to the Ah parent is misclassified into the Ag matrix, the resulting loss is recorded as: L{ g / h }, for the same reason:

$$P(g,h) = \int_{Rh} f_h(x)dx$$

$$W_g = \sum_{h=1,g\neq h}^{G} L\{g/h\}P\{g/h\} = \sum_{h=1,g\neq h}^{G} L\{g/h\}\int_{Rh} f_h(x)dx$$

$$W_R = \sum_{g=1}^{G} q_g = \sum_{h=1,h\neq g}^{G} L\{g/h\}\int_{Rh} f_h(x)dx$$

$$\{R_g\}: \sum_{g=1,g\neq h}^{G} L\{h/g\}q_g f_g(x) > g \sum_{g=1,g\neq h}^{G} L\{h/g\}q_h f_h(x)$$

Bayes proved that to minimize the total error of the total error, the method of dividing the space {R} should satisfy the following inequalities:

$$\{R_g\}: \sum_{g=1,g\neq h}^{G} L\{h/g\}q_g f_g(x) > g \sum_{g=1,g\neq h}^{G} L\{h/g\}q_h f_h(x)$$

That is to say, the individual with the highest posterior probability of the Ag parent is assigned to the A_g parent. The maximum posterior probability is equivalent to the maximum $q_g f_g(x)$, so the discriminant function of any individual X for discriminant attribution can be derived. The available G discriminant functions are:

$$q_g f_g(x) = q_g (2\pi)^{-\frac{p}{2}} |\Sigma^{-1}|^{\frac{1}{2}} \exp\left[-\frac{1}{2}(x-a_g)'\Sigma^{-1}(x-a_g)\right]$$

Where $X=(x_1,x_2,\ldots\ldots,xn)'$, the parameters Ag and Σ are the mean vector and covariance matrix of the parent , respectively, g = 1, 2, ..., G. After derivation and sorting, the normal matrix multi-class linear discriminant function under Bayes criterion can be obtained as:

$$Z(x) = b_{0g} + b_{1g}Y_1 + \cdots + b_{pg}Y_p$$

Finally, compare $Z_1(x)$, $Z_2(x)$, ……, $Z_G(x)$, and select the maximum value to determine the precursor from which sample X is derived (Zhang Dandan 2017).

Results nd Discussions

Hydrochemical Characteristics of Mixed Water

Taking Ordovician limestone and k6-coal 12 aquifer as an example, the simulation results are shown in Table 2.

The result indicates that the concentrations of main ions in the mixed water all showed an decrease tendency with continuously extend of ordovician limestone water. The variation of Na^+, SO_4^{2-}, HCO^{3-} is smoother, K^++Na^+ decreased from 19.5 mg/L to 12.5mg/L, SO_4^{2-} is reduced from 35.8 mg/L to 17.9 mg/L, and HCO^{3-} shifted from 207.2 mg/L to 159.3 mg/L. At the same time, Ca^{2+} is changed from 58.2 mg/L to 47.6 mg/L, and Mg^{2+} is narrowed from 22.7mg/L to 13.7 mg/L. While Cl^- is increased from 11.1 mg/L to 18.1 mg/L, and NO^{3-} is extended from 3.1 mg/L to 27.3 mg/L. In addition, Total Dissolved Solids (TDS) and the mineralization is also gradually decreasing with a large percentage of ordovician limestone water, whereas the total hardness and PH getting bigger.

Analysis of the Bayes discriminant model

Bayes discriminant analysis was performed on 36 water samples of four aquifers infiltrated into the gray water using SPSS statistical analysis software. Five principal component variables(Na^+, Ca^+, Mg^+, SO_4^{2}, CO_3^{2-}) were selected as indicators of the Bayes discriminant analysis model. The coefficient matrix of the Bayes discriminant model is shown in Table 3.

By Bayes discriminant function coefficient matrix, the function expression of Bayes discriminant model can be obtained as follows:

For convenience of writing, replace variables Na^+, Ca^+, Mg^+, SO_4^{2-} and CO_3^{2-} with Y_1, Y_2, Y_3, Y_4, Y_5 in the function expression.

$$\begin{cases} Z_1 = 475.196Y_1 + 1276.769Y_2 + 990.490Y_3 - 1120.524Y_4 - 69.493Y_5 - 23134.172 \\ Z_2 = 473.305Y_1 + 1272.494Y_2 + 987.113Y_3 - 1126.333Y_4 - 69.041Y_5 - 22903.290 \\ Z_3 = 470.708Y_1 + 1263.714Y_2 + 979.490Y_3 - 1117.639Y_4 - 68.865Y_5 - 22634.467 \\ Z_4 = 489.111Y_1 + 1313.858Y_2 + 1019.370Y_3 - 1162.471Y_4 - 71.599Y_5 - 24467.549 \end{cases}$$

Model's back substitution test, pending test and error analysis

According to the discriminant function of Bayes, the sample data is substituted into the above discriminant function for calculation. The data of Z_1, Z_2, Z_3 and Z_4 can be calculated, corresponding to the water source type: k6–coal 12 water, coal 9–coal 7 water, coal

***Table 2** Primary Hydrochemical Data of Water Samples in Jinggezhuang Aquifers*

Mixing ratio	1:9	2:8	3:7	4:6	5:5	6:4	7:3	8:2	9:1
pH	7.68	7.69	7.71	7.72	7.74	7.75	7.77	7.79	7.82
Na^{+} (mg/L)	19.52	18.64	17.77	16.89	16.02	15.14	14.26	13.39	12.51
Ca^{2+} (mg/L)	58.16	56.84	55.52	54.20	52.88	51.56	50.23	48.91	47.59
Mg^{2+} (mg/L)	22.71	21.58	20.45	19.32	18.19	17.06	15.93	14.80	13.67
Fe^{2+} (mg/L)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fe^{3+} (mg/L)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Al^{3+} (mg/L)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NH^{+} (mg/L)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cl^{-} (mg/L)	11.09	11.97	12.85	13.73	14.60	15.48	16.36	17.24	18.11
SO_4^{2-} (mg/L)	35.76	33.53	31.30	29.08	26.85	24.62	22.39	20.16	17.94
HCO^{-} (mg/L)	207.22	201.23	195.25	189.26	183.27	177.28	171.30	165.32	159.33
NO_{3-} (mg/L)	3.10	6.12	9.15	12.18	15.20	18.23	21.26	24.28	27.31
NO_{2-} (mg/L)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

***Table 3** Bayes discriminant coefficient matrix*

Variables	Aquifers			
	K6-coal 12	Coal 9-coal 7	Coal 5 roof sandstone	Quaternary loose alluvium
Na^{+}	475.196	473.305	470.708	489.111
Ca^{+}	1276.769	1272.494	1263.714	1313.858
Mg^{+}	990.498	987.113	979.490	1019.370
SO_4^{2-}	-1128.524	-1126.333	-1117.639	-1162.471
CO_3^{2-}	-69.493	-69.041	-68.865	-71.599
(constant)	-23134.172	-22983.290	-22634.467	-24467.549

***Table 4** Bayes discriminant model backdating test*

K6–coal 12 w		Coal 9–coal 7		Coal 5 sandstone		Alluvial aquifer		Total	
amout	proportion	amout	proportion	amout	proportion	amout	proportion	amout	proportion
9	100%	0	0	0	0	0	0	9	100%
0	0	9	100%	0	0	0	0	9	100%
0	0	0	0	9	100%	0	0	9	100%
1	11.1%	0	0	0	0	8	88.9%	9	100%

Table 5 Bayes discriminant model pending test

K6–coal 12		Coal 9–coal 7		Coal 5 sandstone		Alluvial aquifer		Total	
amout	proportion	amout	proportion	amout	proportion	amout	proportion	amout	proportion
3	100%	0	0	0	0	0	0	3	100%
0	0	3	100%	0	0	0	0	3	100%
0	0	0	0	3	100%	0	0	3	100%
1	33.3%	0	0	0	0	2	66.7%	3	100%

5 sandstone water, alluvial layer water. The maximum value is the type of judged water source. The results of the back-test are shown in Table 4.

The backdating overall correct rate of Bayes discriminant model is 97.2%. The recognition accuracy of k6-coal 12 water, coal 9-coal 7 water and coal 5 water is relatively high, all of which are 100%. One of the water samples is misjudged, accounting for 11.1% of the water samples.

The complex source of alluvial water leads to the unclear hydrochemical characteristics of the aquifer, which results in unsatisfactory linear discriminant effects such as Bayes discriminant analysis.

Conclusions

(1) The concentrations of main ions in the mixed water all showed an decrease tendency with continuously extend of ordovician limestone water. The variation of Na^+, SO_4^{2-}, HCO_{3-} is smoother, K^++Na^+ decreased from 19.5 mg/L to 12.5mg/L, SO_4^{2-} is reduced from 35.8 mg/L to 17.9 mg/L, and HCO_{3-} shifted from 207.2 mg/L to 159.3 mg/L. In addition, Total Dissolved Solids (TDS) and the mineralization is also gradually decreasing with a large percentage of ordovician limestone water, whereas the total hardness and PH getting bigger.

(2) Bayes discriminant analysis was carried out by SPSS statistical analysis software, and the discriminant model was obtained. The overall accuracy of Bayes discriminant model is 91.7%. It is expected to provide a scientific basis for rapid identification of mine water inrush sources.

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Conflicts of Interest:

The authors declare no conflict of interest.

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