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Application of Chemical Dynamics Method in Solving Hydro-Geological Parameters

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Abstract

With the increasing of coal mining depth, the coal seam floor is threatened more and more seriously with the limestone aquifer of Taiyuan Formation. In order to make the coal seam floor water inrush accident to be effectively prevented, it is very important to ascertain the hydro-geological condition of the research area and adequately gain hydro-geological parameters. Based on the theory of chemical dynamics, the chemical dynamical equation of the mineral was obtained. The chemical dynamical equation of the mineral and the Darcy's Law were combined to derive the expression of permeability coefficient and transmissibility coefficient that was indicated by hydro-chemistry index. Based on the data of water quality analysis in the research area, the hydro-geology parameter of the aquifer of Taiyuan Formation was calculated. And it was compared with what the hydro-geology parameter was determined by the data of pumping test. The results show that the permeability coefficient (K) of the research area is 1.7512 m/d, and transmissibility coefficient (T) is 42.0282 m^2/d. The calculated results of chemical dynamics and pumping test results are little different between them. And it has certain practical significance in the mine water control. It provides an effective method for obtaining hydro-geological parameters.

Keywords

Hydro-Geology Parameter, Chemical Dynamics Equations, Permeability Coefficient, Transmissibility Coefficient

1. Introduction

With the increasing demand for coal resources in China, the work of coal mining is gradually developed into the deep mining depth and complex geological conditions [1] [2] [3] [4]. The continuous increase of mining depth has become the main method of mining. Along with the continuous increase of mining depth, the Mining under Pressure has become the main method of mining. And the threat of coal seam mining will gradually aggravate from the depth of the aquifer of Taiyuan Formation. The safety of coal seam floor is very important [1] [2] [3]. The main reason is the complex geological and hydro-geological conditions of aquifer and insufficient understanding of hydro-geological conditions. Meanwhile, it is difficult to obtain the basic hydro-geological parameters. Therefore, it is of great practical significance to identify the aquifer properties and hydro-geological parameters of the coal seam floor before mining, which is of the most importance for the prevention and control of water in coal mines [3] [4] [5] [6].

For a long time, many methods were usually used in the process of obtaining hydro-geological parameters. For example, pumping test, slug test, water pressure test and so on [4] [5]. According to Zhang H.Y. *et al.* [6], taking the South deep mining area of the Chensilou coal as the research object, the hydro-geological parameters of limestone aquifer were calculated by unsteady flow dewatering test. According to Ju X.M. *et al.* [7], the pumping tests and slug tests at the same time in the Laosui river of Huaibei in Anhui province were carried out, and the results of the two methods were compared and analyzed. According to Hu W.Y. *et al.* [8], a simple method of calculating hydro-geological parameters was introduced by the observed dynamic data of ground water level for a long time. These methods of obtaining hydro-geological parameters could be summarized as hydrodynamic methods [4]-[9]. In recent years, experts and scholars have put forward the method of chemical dynamics to obtain hydro-geological parameters [10]-[15] and the quantitative evaluation of hydro-geological conditions in the study area is realized.

On this basis, this paper took a mine in Anhui province as an example. The expression of hydro-geological parameters was derived by using the method of Chemical Dynamics. And the hydro-geology parameter of the limestone aquifer of Taiyuan Formation was calculated. The data of pumping test in the research area was collected and arranged. The calculated results of chemical dynamics and pumping test results were compared to analyze the reason for the deviation.

2. Chemical Dynamics Parameters

2.1. Determination of Ion Activity

In the ground water, part of the ions does not work in the reaction process due to the interaction of various ions. This leads to a difference between the effective concentration of the ions and the true concentration of the ions in the process of chemical reaction [10] [11] [12] [14]. Therefore, it is necessary to correct the measured concentration in the ground water. The corrected concentration is known as the Ion Activity and is represented by α_i. The Relationship between Ion Activity (α_i) and the true concentration of the ions (c_i) is as follows [10]:

$$\alpha_i = \gamma_i \times c_i \tag{1}$$

where, γ_i is the activity coefficient.

At this time the theory of Debye and Hükel is used to explain difference between the ground water solution and ideal solution. And the formula for calculating the activity coefficient of an ion solution by mathematical method is as follows [10] [11]:

$$\lg \gamma_i = -\frac{A z_i^2 \sqrt{I}}{1 + B a_i \sqrt{I}} \tag{2}$$

where, A and B are constants that depend on the temperature of the water. a_i is constant that depends on the ionic radius. I is the ionic strength of the solution.

The ionic strength (I) is a measure of the electrostatic field that formed by various ions in the solution. And the formula for calculating the ionic strength (I) is as follows:

$$I = \frac{1}{2} \sum_{i=1}^{M} m_i z_i^2$$

where, m_i is the substance concentration of the ion. z_i is the Valence number of ion. M is the kinds of ion.

The theory of Debye and Hükel was applied to the temperature of 0 to 60. The values of A and B are as follows.

According to the data in **Table 1**, the curve fitting of T with A and B was made. The curve fitting is as follows (**Figure 1**).

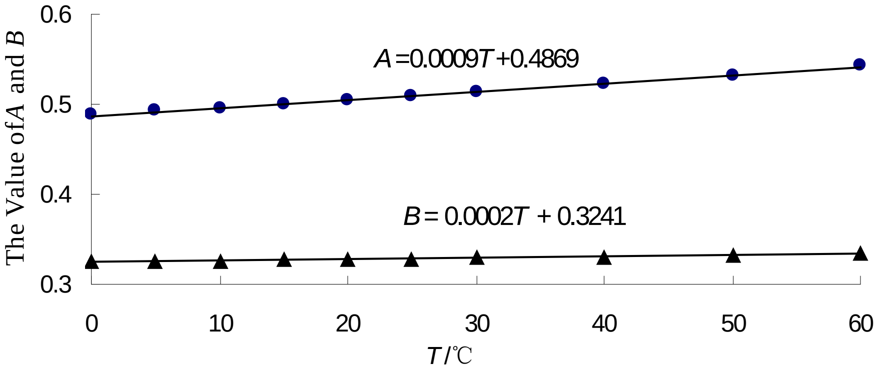

Figure 1. The curve fitting of T with A and B.

Table 1. The value of A and B in different temperature.

T/°C	A	B
0	0.4883	0.3241
5	0.4921	0.3249
10	0.4960	0.3258
15	0.5000	0.3262
20	0.5042	0.3273
25	0.5085	0.3281
30	0.5130	0.3290
40	0.5221	0.3305
50	0.5319	0.3321
60	0.5425	0.3338

2.2. Determination of Saturation Index

The Saturation index is a parameter to determine the state of water and minerals, and is an important means to evaluate the formation and development of karst. It is expressed by the symbol of SI. When $SI > 0$, it means that the mineral is in a super-saturation state. When $SI = 0$, it means that the mineral is in a saturation state. When $SI < 0$, it means that the mineral is in a dissolved condition.

The multi mineral system refers to the dissolution of calcite, dolomite, and gypsum in the CO_2-H_2O system. Under these circumstances, the saturation index is calculated by the mineral composition of ion activity and solubility product constant. The saturation index of Calcite, Dolomite and Gypsum are as follows:

$$\left.\begin{aligned} \beta_c &= \left(K_2 \alpha_{\mathrm{Ca}^{2+}} \cdot \alpha_{\mathrm{HCO}_3^-}\right) \Big/ \left(K_c \cdot \alpha_{\mathrm{H}^+}\right) \\ \beta_d &= \left(K_2 \alpha_{\mathrm{Ca}^{2+}} \cdot \alpha_{\mathrm{Mg}^{2+}} \cdot \alpha^2_{\mathrm{HCO}_3^-}\right) \Big/ \left(K_d \alpha^2_{\mathrm{H}^+}\right) \\ \beta_g &= \left(\alpha_{\mathrm{Ca}^{2+}} \cdot \alpha_{\mathrm{SO}_4^{2-}}\right) \Big/ K_g \end{aligned}\right\} \tag{3}$$

where, a_i is the ion activity of i, K_1 is the first-order dissociation constant of carbonic acid, K_2 is the second-order dissociation constant of carbonic acid, K_c is the dissociation constant of Calcite, K_d is the dissociation constant of Dolomite, K_g is the dissociation constant of Gypsum.

3. Calculation of Hydro-Geological Parameters

3.1. The Darcy's Law Is Expressed by Chemical Indexes

If the component of i is generated through many minerals, the equation of the mineral dissolution process can be superimposed. In some monographs [10] [12] [16] [17] [18], according to the theory of chemical dynamics, the chemical dynamics equation for the dissolution of minerals was derived. And the equation is as follows:

$$\frac{\mathrm{d}a_{ij}}{\mathrm{d}t} = \sum_{j=1}^{m} v_{ij} k_j \left(1 - \beta_j\right) \tag{4}$$

The Equation (4) was deformed as follows:

$$\frac{\mathrm{d}s_i}{\mathrm{d}t} \cdot \frac{\mathrm{d}a_{ij}}{\mathrm{d}s_i} = \sum_{j=1}^{m} v_{ij} k_j \left(1 - \beta_j\right) \tag{5}$$

In the process of ground water movement, the $\mathrm{d}s_i/\mathrm{d}t$ can be considered as the infiltration velocity (V_{ni}) on the groundwater flow line. If V_{ni} is substituted into Equation (5), it will get the following relationship:

$$V_{ni} \cdot \frac{\mathrm{d}a_{ij}}{\mathrm{d}s_i} = \sum_{j=1}^{m} v_{ij} k_j \left(1 - \beta_j\right) \tag{6}$$

$$V_{ni} = \frac{\sum_{j=1}^{m} v_{ij} k_j \left(1 - \beta_j\right)}{\mathrm{d}\alpha_{ij} / \mathrm{d}S_i} = \frac{\left[\sum_{j=1}^{m} v_{ij} k_j \left(1 - \beta_j\right)\right] \mathrm{d}S_i}{\mathrm{d}\alpha_{ij}} \tag{7}$$

where, j is the number of dissolved mineral, i is the component of ion from mineral dissolution, V_{ni} is the infiltration velocity of the component of i on the groundwater flow line, a_{ij} is the ion activity of the component of i from the mineral of j, S_i is the flow distance of the component of i along with the stream line, v_{ij} is the stoichiometric number of the component of i that dissolve from the mineral of j, k_j is the chemical dynamics constant for the dissolution of mineral of j.

Because of the ion activity (α_i) and the saturation index (β_j) are the functions of time and space, the Equation (7) can be integrated. It will get the following relationship:

$$V_{ni}\int_{\alpha_{ijA}}^{\alpha_{ijB}} \mathrm{d}\alpha_{ij} = \int_{S_{iA}}^{S_{iB}}\left[\sum_{j=1}^{m} v_{ij}k_j\left(1-\beta_j\right)\right]\mathrm{d}S_i \tag{8}$$

The Equation (8) can be simplified by using the trapezoid formula. The Equation (8) was deformed as follows:

$$V_{ni} = \frac{\Delta S_{iAB}\sum_{j=1}^{m} v_{ij}k_j\left(2-\beta_{jA}-\beta_{jB}\right)}{2\Delta\alpha_{ijAB}} \tag{9}$$

where, ΔS_{iAB} is the flow distance of the component of i from A to B, $\Delta\alpha_{ijAB}$ is the ion activity of the component of i from A to B, β_{jA} is the saturation index of the mineral of j at A, β_{jB} is the saturation index of the mineral of j at B.

3.2. Expression of Hydro-Geological Parameters

If Equation (9) is substituted into the expression of the Darcy's Law that is expressed by Hydraulic index, it will get the following relationship:

$$K_{AB} = \frac{V_{nijAB}}{I_{iAB}} = \frac{\Delta S_{iAB}^2\sum_{j=1}^{m} v_{ij}k_j\left(2-\beta_{jA}-\beta_{jB}\right)}{2\Delta\alpha_{ijAB}\Delta h} \tag{10}$$

$$T_{AB} = \frac{V_{nijAB}}{I_{iAB}} = \frac{\Delta S_{iAB}^2\sum_{j=1}^{m} v_{ij}k'_j\left(2-\beta_{jA}-\beta_{jB}\right)}{2\Delta\alpha_{ijAB}\Delta h} \tag{11}$$

$$k'_j = k_j \cdot M \tag{12}$$

where, K_{AB} is the permeability coefficient, Δh is the height deviation between A and B. M is thickness of the limestone aquifer of Taiyuan Formation.

3.3. Expression of Chemical Dynamics Constant

There are two methods for obtaining chemical dynamics constants, which are laboratory test and field test. The chemical dynamics constants were obtained by taking field experiments in this paper. And the equation is as follows:

$$k_j = \frac{2\bar{K}\Delta h_{AB}\Delta a_{ijAB}}{\Delta S_{AB}^2\left(2-\beta_{jA}-\beta_{jB}\right)} \tag{13}$$

where, $\bar{K}$ is the permeability coefficient that was obtained by hydraulic index. According to the results of pumping test in the study area, the $\bar{K}$ is equal to 1.3913 m/d.

On the basis of the chemical dynamics constants was obtained by predecessors, the chemical dynamics constants of Calcite, Dolomite and Gypsum were calculated respectively. The corresponding permeability coefficient (K) and transmissibility coefficient (T) were obtained by using the chemical dynamics constants of Calcite, Dolomite and Gypsum. Then the average of permeability coefficient (K) and transmissibility coefficient (T) were calculated.

The chemical dynamics constants of Calcite (c), Dolomite (d) and Gypsum (g) are expressed as follows:

$$\left.\begin{aligned} k_c &= \frac{2\bar{K}\Delta h_{AB}\left(\Delta\alpha_{\mathrm{Ca}^{2+}} - \Delta\alpha_{\mathrm{Mg}^{2+}} - \Delta\alpha_{\mathrm{SO}_4^{2-}}\right)}{\Delta S_{AB}^2\left(2-\beta_{cA}-\beta_{cB}\right)} \\ k_c' &= k_c \cdot M \end{aligned}\right\} \tag{14}$$

$$\left.\begin{aligned} k_d &= \frac{2\bar{K}\Delta h_{AB}\Delta\alpha_{\mathrm{Mg}^{2+}}}{\Delta S_{AB}^2\left(2-\beta_{dA}-\beta_{dB}\right)} \\ k_d' &= k_d \cdot M \end{aligned}\right\} \tag{15}$$

$$\left.\begin{aligned} k_g &= \frac{2\bar{K}\Delta h_{AB}\Delta\alpha_{\mathrm{SO}_4^{2-}}}{\Delta S_{AB}^2\left(2-\beta_{gA}-\beta_{gB}\right)} \\ k_g' &= k_g \cdot M \end{aligned}\right\} \tag{16}$$

3.4. The Calculation of Hydro-Geological Parameters by Chemical Indexes

The research area is located in the south of the mine field. The main aquifers include the first to fourth aquifer of Cenozoic Erathem, the sandstone aquifers in coal measures and the limestone aquifer of Taiyuan Formation. The aquifer in the research area is shown in **Figure 2**. The limestone aquifer of Taiyuan Formation is one of the major hidden dangers of mine filling water. And it is of great significance to research the limestone aquifer of Taiyuan Formation.

A total of 10 water samples were taken at 1 to 5# sampling points in the research area, and there are 2 water samples at each sampling point. The 10 water samples were used for water quality analysis. The distributions of sampling points are shown in **Figure 3**. The results of water quality analysis are shown in **Table 2**.

According to the geological report of the research area, the thickness of the limestone aquifer of Taiyuan Formation is 24 meters. So, the chemical dynamics constant could be calculated by Equation (14), Equation (15) and Equation (16). The results are shown in **Table 3**.

Meanwhile, the permeability coefficient (K) and transmissibility coefficient (T) were calculated by Equation (10), Equation (11) and Equation (12). It can be listed in **Table 4**.

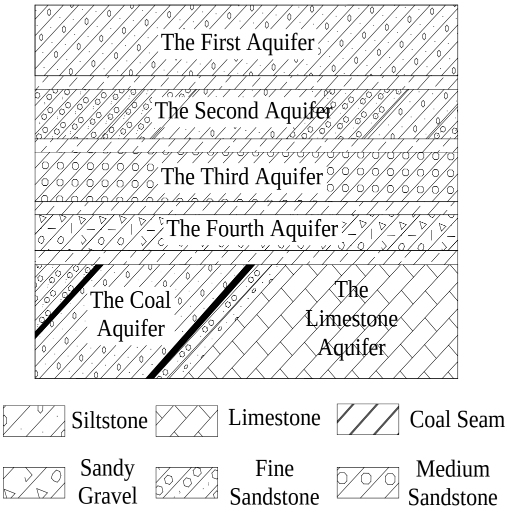

Figure 2. The aquifer in the research area.

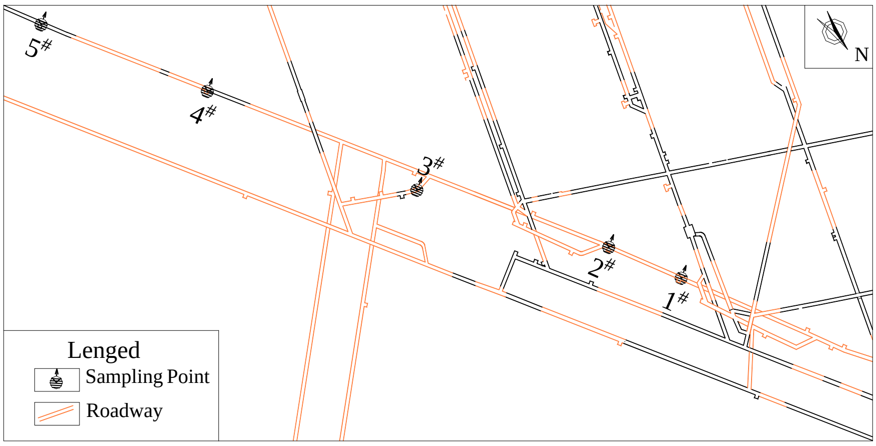

Figure 3. The distribution of sampling point.

Table 2. The results of water quality analysis.

Sampling Point	No.	The Content of Ions (mg/L)							pH
		Cl^-	SO_4^{2-}	HCO_3^-	CO_3^{2-}	$Na^+ + K^+$	Ca^{2+}	Mg^{2+}	
$1^{\#}$	1	278	667	428.17	5.17	276.9	214	81.5	7.32
	2	243	614	430.56	5.32	254.5	198	78.1	7.27
$2^{\#}$	3	265	606	428.17	4.19	270.7	215	82.9	7.33
	4	255	619	394.68	4.53	258.4	201	79.3	7.45
$3^{\#}$	5	262	608	425.77	5.95	269.9	209	80.5	7.41
	6	248	596	428.17	5.36	256.4	201	76.1	7.27
$4^{\#}$	7	252	349	576.47	5.25	386.5	109	46.4	7.31
	8	231	376	552.55	5.38	371.4	98	45.4	7.28
$5^{\#}$	9	241	404	516.67	4.96	327.4	134	58	7.41
	10	244	600	428.17	4.89	287.2	167	79.2	7.35

Table 3. The chemical dynamics constant.

No.	Calcite		Dolomite		Gypsum	
	k_c	k'_c	k_d	k'_d	k_g	k'_g
A	7.4002×10^{-4}	1.776×10^{-2}	3.6754×10^{-4}	8.8209×10^{-2}	2.4898×10^{-4}	5.9755×10^{-2}
B	1.7354×10^{-5}	4.1649×10^{-4}	6.7415×10^{-5}	1.6179×10^{-3}	2.8497×10^{-5}	6.8393×10^{-4}
C	4.7254×10^{-4}	1.1341×10^{-2}	2.8667×10^{-3}	6.8801×10^{-2}	2.1395×10^{-4}	5.1348×10^{-3}
D	8.0185×10^{-5}	1.9244×10^{-3}	8.6477×10^{-4}	2.0754×10^{-2}	2.5215×10^{-5}	6.0516×10^{-3}

Table 4. The calculation of hydro-geological parameters

No.	Permeability Coefficient (m/d)	Transmissibility Coefficient (m^2/d)
A	1.3913	33.3912
B	1.6942	40.6608
C	1.9203	46.0872
D	1.9989	47.9736
Average Value	1.7512	42.0282

The contour map of the permeability coefficient in the research area is shown as follows.

3.5. Evaluation of Hydro-Geological Conditions

It can be seen from **Figure 4** that the permeability coefficient of the limestone aquifer of Taiyuan Formation in the whole research area has little change in general. According to the results of the hydro-geological parameters in **Table 4**, we can know that the permeability coefficient in research area is equal to 1.7512 m/d and the transmissibility coefficient is equal to 42.0282 m^2/d. According to classification standard of permeability coefficient and transmissibility coefficient, it can be concluded that the limestone aquifer of Taiyuan Formation has strong water permeability and medium water conductivity. According to the results of pumping test, the permeability coefficient is 1.3913 m/d and the transmissibility coefficient is 33.3912 m^2/d. The comparison between the results of the pumping test and the hydro-geological parameters of the water chemistry index shows that the permeability coefficient and the conductivity coefficient are not significantly different. To a degree, it is reliable that the results of hydro-geological parameters were obtained by water chemistry index. It also provides a new method for the evaluation of hydro-geological condition.

4. Conclusions

1) The results show that the limestone aquifer of Taiyuan Formation has strong water permeability and medium water conductivity, and the hydro-geological parameters of the whole research area have not changed much.

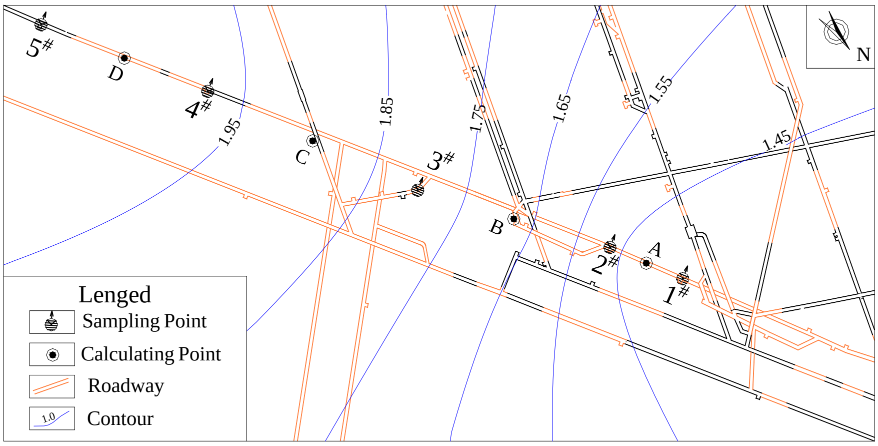

Figure 4. Contour map of permeability coefficient.

2) The little difference between the hydro-geological parameters was obtained by the chemical dynamics method and was obtained from the pumping test. It shows that it is feasible to evaluate hydro-geological condition from the point of view of chemical dynamics. And the chemical dynamics has a certain application prospect.

3) In order to improve the accuracy of the calculation of hydro-geological parameters by chemical dynamics method, the following points should be made in the following work: a) More water samples are collected for water quality analysis; b) The sampling points should be evenly distributed in time and space; c) The retrieved water samples should be immediately analyzed for water quality to avoid evaporation of water and affect the results of water quality analysis; d) Water samples were collected for water quality analysis to reduce test errors.

Acknowledgements

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