Study on Water Quality Evolution of Water Inrush from Typical Coal Mine Roof Cretaceous Aquifer in WesternChina Mining Area

Jia Ding[1,2], Shuning Dong[1,2], Xiaoming Guo[1,2], Feng Liu[1,2], Wenzhong Zhang[1,2]

[1]*CCTEG Xi'an Research Institute (Group) Co., Ltd., Xi'an 710077, China*

[2]*State Key Laboratory of Coal Mine Disaster Prevention and Control, Xi'an 710077, China*

Abstract

To clarify the hydrogeochemical evolution mechanism of roof inflow water in Cretaceous aquifers of western China coal mines, this study takes Dafosi Coal Mine as the research object, combining field sampling, laboratory testing and PHREEQC geochemical modeling to analyze the water-rock interaction process during the migration of Luohe Formation aquifer water through Jurassic strata to the mining face. The results show that silicate mineral dissolution and cation exchange are the dominant processes altering inflow water quality: Ca^{2+}/Mg^{2+} in groundwater are adsorbed by clay minerals and exchanged with Na^+, leading to a sharp increase in Na^+ and a significant decrease in Ca^{2+}/Mg^{2+}; silicate weathering consumes CO_2/H^+, keeping water slightly alkaline and increasing TDS by ~50%. The water type evolves from HCO_3–Mg·Na·(Ca) to HCO_3–Na (actual inrush water is $HCO_3 \cdot SO_4$–Na). A field roof water inrush event verifies the simulation results, and neglecting such evolution will reduce the reliability of traditional static hydrochemical fingerprint methods for water source identification. It is recommended to incorporate water quality evolution analysis into mine water hazard assessment.

Keywords: Western China coal mine; cretaceous aquifer; roof water inflow; hydrogeochemical evolution; water-rock interaction; PHREEQC

Introduction

Coal is the core energy source for China's energy security, and mining activities are accelerating westward with the depletion of eastern coal resources (Wu *et al.* 2022). Western China coal basins are faced with complex hydrogeological conditions, and roof water inrush from Cretaceous Luohe Formation sandstone aquifers above Jurassic coal seams has become a major hidden danger restricting safe mining (Zeng *et al.* 2023).

Rapid and accurate identification of water inrush sources is the key to mine water hazard control (Motyka *et al.* 2024). Traditional methods rely on the static "hydrochemical fingerprint" of aquifers, but groundwater undergoes continuous water-rock interaction during migration along fracture paths in mining environments, leading to dynamic changes in chemical composition (Jiang *et al.* 2024). In the Ordos Basin and other western mining areas, Luohe Formation groundwater migrates downward through Jurassic strata after the roof fracture zone is connected, and its hydrochemical characteristics are altered by dissolution and ion exchange (Hao *et al.* 2021; Samborska-Goik *et al.* 2024), which may cause misidentification of water sources if ignored.

This study selects Dafosi Coal Mine (Binchang mining area, Shaanxi Province) with typical Cretaceous roof water inrush as the research site, collects water/rock samples for laboratory analysis, and uses PHREEQC to simulate the hydrochemical evolution process. The research results provide a scientific basis for the accurate identification of roof water inrush sources in western China coal mines.

Study Area and Hydrogeological Setting

Dafosi Coal Mine is located in the southern Binchang mining area of the Huanglong Jurassic coal basin, a national high-risk area for mine water disasters. The mine mainly mines the No.4 coal seam of the Jurassic Yan'an Formation at a depth of ~400 m, with prominent roof water inrush hazard from the Cretaceous Luohe Formation.

The study area has a layered aquifer system, and the Huanhe Formation aquitard effectively isolates the shallow Quaternary aquifer, so the roof inflow water is mainly from the Cretaceous Luohe Formation aquifer directly overlying the Jurassic coal measures (Fig.1). The Luohe Formation is composed of loosely cemented sandstone with high porosity, permeability and water yield capacity; the underlying Jurassic strata (Anding, Zhiluo, Yan'an Formations) are fractured and easy to cave in during mining.

When the No.4 coal seam is mined, the roof forms a caved zone and a fissure zone. Once the fissure zone is connected with the Luohe aquifer, pressurized groundwater migrates downward along fractures through Jurassic strata to the mining face, and undergoes full water-rock interaction with broken rock mass during migration, leading to hydrochemical changes. This hydrogeological characteristic makes Dafosi Coal Mine an ideal object for studying water quality evolution of roof inflow water.

Materials and Methods

Sampling and Laboratory Analysis

Groundwater sampling was carried out in the pre-drained borehole above the 40203 longwall panel of Dafosi Coal Mine on March 20 and 22, 2025. After sufficient purging, samples were filtered, stored and acidified in aliquots, and in-situ pH/temperature were measured. Cations (K^+, Na^+, Ca^{2+}, Mg^{2+}) were determined by ICP-OES, anions (Cl^-, SO_4^{2-}, HCO_3^-) by ion chromatography, and HCO_3^- was cross-checked by titration. The average values of the two samples were taken as the initial hydrochemical data (Tab.1).

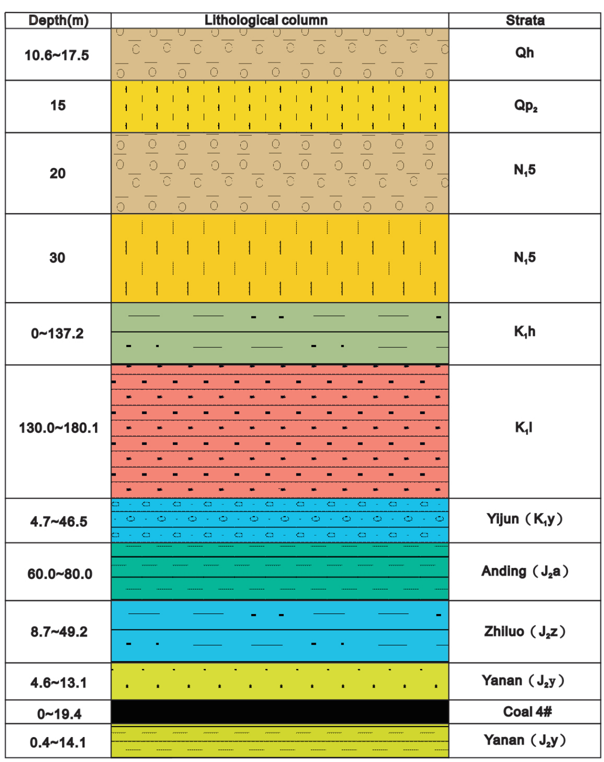
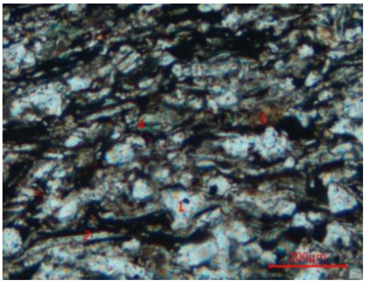
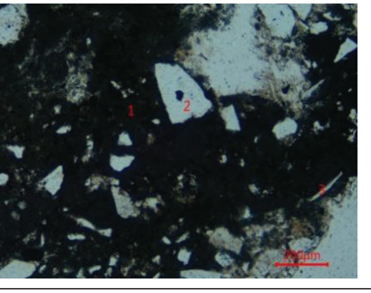


***Figure 1** Generalized hydrogeological column of Dafosi Coal Mine area.*

Table 1 Major ion concentrations of Luohe Formation aquifer water.

Date	K^+ (mg/L)	Na^+ (mg/L)	Ca^{2+} (mg/L)	Mg^{2+} (mg/L)	Cl^- (mg/L)	SO_4^{2-} (mg/L)	HCO^{3-} (mg/L)	TDS (mg/L)	pH
2025/03/20	1.16	53.18	32.36	30.63	6.12	347.24	347.24	516.53	8.00
2025/03/22	1.56	74.2	34.18	31.89	32.65	308.57	308.57	551.75	8.22
Average	1.36	63.69	33.27	31.26	19.385	50.99	327.905	534.14	8.11

Table 2 Mineral composition of roof strata rock samples (Only a portion is displayed due to space constraints).

Sample number	X-ray diffraction analysis results	Mineral composition and content
		Clay minerals ~45% Muscovite ~30% Quartz ~15% Mica ~6% Chlorite ~4% Metal minerals <1%
		Clay minerals ~70% Muscovite ~3% Quartz ~10% Sericite ~12% Chalcedony ~4% Calcite ~1%

Eight representative core samples were collected from the Jurassic Anding/Zhiluo Formations between the Luohe aquifer and the No.4 coal seam. XRD analysis was performed on air-dried and crushed samples to determine mineral composition. The results show that the roof strata are dominated by silicate minerals: clay minerals (illite/chlorite) account for 45%~85% of most samples (strong cation exchange capacity), followed by quartz (10%~50%), with small amounts of muscovite, feldspar and trace calcite cement. The high clay content provides material conditions for water-rock interaction.

Geochemical Modeling

PHREEQC hydrogeochemical simulation software was used to construct the reaction path model of Luohe aquifer water reacting with Jurassic roof rocks. The initial solution was the average hydrochemical composition of Luohe aquifer water, and the reaction mineral phases included illite, chlorite, K-feldspar, plagioclase, quartz, calcite and pyrite (based on XRD results, Tab 2).

The model set reaction control conditions: calcite/gypsum for equilibrium dissolution-precipitation, silicate minerals for kinetic dissolution (literature rate parameters), and clay surface cation exchange for equilibrium reaction (literature ion exchange capacity). The simulation was carried out with reaction progress from 0 (initial aquifer water) to 1 (full equilibrium with rock mass), and the changes of pH, major ion concentration and TDS were calculated to identify the dominant geochemical processes and water chemistry evolution trends.

Results and Discussion

Simulated Water Chemistry Evolution by Water-Rock Interaction

PHREEQC simulation results show that silicate mineral dissolution and cation exchange are the two dominant geochemical processes driving hydrochemical evolution, and water chemistry indicators change regularly with reaction progress. Cation exchange is the core process of cation composition change: Na^+ concentration rises sharply from 63.69 mg/L to ~230 mg/L, while Ca^{2+} and Mg^{2+} decrease to near zero. The essence is the exchange between Ca^{2+}/Mg^{2+}in water and Na^+ on clay minerals, with the reaction equation:

Silicate mineral dissolution releases K^+/Na^+ and produces H_4SiO_4, and its weathering consumes H^+/CO_2 to generate additional HCO_3^-, keeping HCO_3^- concentration high and water slightly alkaline (pH rises from 8.11 to 8.2~8.7). Ion release from cation exchange and silicate dissolution leads to a ~50% increase in TDS (from 534.14 mg/L to ~795 mg/L). With the progress of water-rock interaction, the original HCO_3–Mg·Na·(Ca) type water gradually evolves into HCO_3–Na type water with high Na^+, high SiO_2, low $Ca^{2+}$and low Mg^{2+}.

Field Validation by Roof Water Inrush Event

On October 15~16, 2024, a roof water inrush event occurred in the 40103 longwall panel of Dafosi Coal Mine (maximum inflow ~200 m^3/h). Water samples were collected from the fault inflow point for hydrochemical testing, and the results were compared with the simulation data and original aquifer water characteristics, as shown in Tab. 3.

The hydrochemical characteristics of actual inrush water are highly consistent with the simulation results: Na^+ concentration increases sharply, Ca^{2+}/Mg^{2+} decrease significantly (Mg^{2+} is nearly completely depleted), pH rises and TDS increases by ~50%. The actual water type is HCO_3·SO_4–Na, and the high SO_4^{2-} is related to pyrite oxidation under mining disturbance and residual pore water

Table 3 *Comparison of hydrochemical characteristics of original aquifer water.*

Index	Initial aquifer water sample (simulation initial)	Simulate the water sample after the reaction	Actual water sample(2024/10/16)
Hydrochemical type	HCO_3-Mg·Na·(Ca)	HCO_3-Na	HCO_3·SO_4-Na
pH	8.11	8.72	8.68
TDS (mg/L)	534	795	813~819
Na^+ (mg/L)	63.7	233	233~240
Ca^{2+} (mg/L)	33.3	9.1	6.5~11.6
Mg^{2+} (mg/L)	31.3	1.4	1.1~1.5
K^+ (mg/L)	1.36	2.5	2.3~2.7
HCO_3^- (mg/L)	328	330	333~335
Cl^- (mg/L)	19.4	19(initial)	52~67
SO_4^{2-} (mg/L)	51.0	51(initial)	116~141

mixing in Jurassic strata. The consistency verifies the reliability of the simulated water-rock interaction process and evolution trend.

Impact on Mine Water Source Identification

The hydrochemical evolution of roof inflow water has a critical impact on traditional static hydrochemical fingerprint identification: the original Luohe aquifer water is HCO_3–Mg·Na·(Ca) type, while the actual inrush water is HCO_3·SO_4–Na type with high Na^+ and low Ca^{2+}/Mg^{2+}. If the evolution process is ignored, the hydrochemical characteristics of inrush water will be inconsistent with the aquifer baseline data, which may lead to misjudgment that the inrush water is a mixture of Luohe aquifer and other deep aquifers.

In western China Jurassic coal mines with developed roof fractures and strong water-rock interaction, the aquifer hydrochemical fingerprint is a dynamic characteristic changing with groundwater migration. The traditional direct comparison method is difficult to meet the accuracy requirements, and it is necessary to incorporate hydro-geochemical evolution analysis into the identification system and combine geochemical modeling to predict water chemistry variation, so as to improve the reliability of water source identification.

Conclusions

The original water of the Cretaceous Luohe Formation aquifer in Dafosi Coal Mine is HCO_3–Mg·Na·(Ca) type with moderate mineralization (TDS=534.14 mg/L) and slightly alkaline (pH=8.11). The Jurassic roof strata are dominated by clay minerals (illite/chlorite) with high cation exchange capacity, which provides the material basis for water-rock interaction. Silicate mineral dissolution and cation exchange are the dominant geochemical processes of water quality evolution: cation exchange leads to a sharp increase of Na^+ and a significant decrease of Ca^{2+}/Mg^{2+}; silicate weathering maintains the slight alkalinity of groundwater (pH=8.2~8.7) and increases TDS by about 50%, and the water type evolves to HCO_3–Na type with high SiO_2 content.

The field roof water inrush event verifies the simulation results: the inrush water is HCO_3·SO_4–Na type, with Na^+ increased to 233.33 mg/L, Ca^{2+}/Mg^{2+} decreased to 9.09/1.36 mg/L, TDS increased to 795.23 mg/L and pH rose to 8.72, which is highly consistent with the predicted evolution trend. Neglecting hydrogeochemical evolution will reduce the accuracy of traditional static hydrochemical fingerprint methods. For western China coal mines with complex hydrogeological conditions, it is necessary to incorporate water quality evolution analysis into mine water hazard assessment and combine geochemical modeling to predict the dynamic variation of water chemistry, so as to improve the reliability of water inrush source identification and the scientificity of mine water hazard prevention and control.

References

Wu M, Hu N, Ye Y, *et al* (2022) Multi-hazard risk characterization and collaborative control oriented to space in non-coal underground mines. Scientific Reports 12:. https://doi.org/10.1038/s41598-022-20437-8

Zeng Y, Mei A, Wu Q, *et al*. Double verification and quantitative traceability for mixed mine water sources[J]. Journal of Hydrology, 2024, 630: 130725.

Motyka J, Cień D, d'Obyrn K. The Use of Hydrochemical Zoning to Predict Water Hazards[J]. Mine Water and the Environment, 2024, 43(2): 198-209.

Jiang Y, Liu H, Liang T, *et al* (2024) Impact of water-rock interaction on natural fractures and shale permeabilities under the closure stress. Geoenergy Science and Engineering 243:213357. https://doi.org/10.1016/j.geoen.2024.213357

Hao C, Gui H, Sheng L, *et al* (2021) Contrasting water–rock interaction behaviors of antimony and arsenic in contaminated rivers around an antimony mine, Hunan Province, China. Geochemistry 81:125748. https://doi.org/10.1016/j.chemer.2021.125748

Rivas S, Sanchez-Alfaro P, Alvarez-Amado F, *et al* (2024) Water-rock interaction and magmatic contribution in thermal fluids of the Southern Volcanic Zone, Chile: Insights from Li, B and Sr isotopes. Journal of Volcanology and Geothermal Research 453:108149. https://doi.org/10.1016/j.jvolgeores.2024.108149

Samborska-Goik K, Ulańczyk R, Krupanek J, Pogrzeba M (2024) A PHREEQC-Based Tool for Planning and Control of In Situ Chemical Oxidation Treatment. Applied Sciences 14:3600. https://doi.org/10.3390/app14093600