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Hydrogeochemical constraints on coalbed methane productivity control mechanism: synergistic effects of fracturing fluid contamination identification and reservoir dynamic response

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Abstract

Accurate identification of geochemical features in coalbed methane (CBM) well-produced water is vital for evaluating the gas potential of reservoirs. However, fracturing fluid interference with water chemistry and productivity analysis is a challenge. This study reveals the origin of produced water ions and their control mechanisms on productivity in CBM wells, based on hydrochemical data from 31 CBM wells in the Gujiao Block, Xishan Coalfield, China. To extract original reservoir information, we established quantitative identification criteria for fracturing fluid contamination ($\text{Cl}^- < 70 \text{ meq/L}$ and $\text{K}^+ + \text{Ca}^{2+} + \text{Mg}^{2+} < 2.5 \text{ meq/L}$), effectively excluding 29% of contaminated samples. Analysis of the water origin and system conditions indicated that the dominant Cl-Na water results from salt dissolution and cation exchange. Ba^{2+} - Sr^{2+} enrichment reflects a marine-terrestrial transitional environment in the Taiyuan Formation, while δD - $\delta^{18}\text{O}$ indicates slow water circulation, with CBM water mainly sourced from sandstone. The produced water in the study area mainly comes from the Member 3 Formation sandstone aquifer. The synergistic effects of SrSO_4 - BaSO_4 precipitation in microfractures, as well as the enrichment and fractionation of hydrogen and oxygen isotopes in high hydrodynamic zones, are the main controlling factors for low productivity. Under weak hydrodynamics, cation exchange, microbial dissolution, sulfate reduction, and CO_2 dissolution enrich Na^+ - HCO_3^- -TDS- Li^+ , enhancing gas well productivity. Ultimately, by integrating these hydrochemical parameters, the ion evolution pathways in wells with different production capacities were analyzed, and a geochemical mechanism model for CBM water production control was constructed. This research provides a crucial hydrochemical evaluation basis for the efficient development of CBM.

Keywords Coalbed methane · Hydrochemistry · Isotopes · Water source identification · Productivity response · Gujiao block

Introduction

Groundwater serves as the medium for natural gas generation and storage, as well as being an essential carrier for natural gas transportation. Groundwater interacts with the aquifer medium in its surrounding environment over long geological periods, resulting in varying chemical compositions. These compositions record reservoir information to varying degrees (Wang et al. 2015; Zhou et al. 2020; Yang et al. 2019; Hosseini 2023). During the coalbed methane (CBM) production, it is necessary to depressurize the coal reservoir by discharging groundwater from the coal seam and surrounding strata in order to facilitate the desorption of methane (Chen et al. 2023; Dai et al. 2023; Arif et al. 2024). Hence, the analysis of ionic composition, contributes to the prediction of the production potential of CBM wells by determining the sources of ions and the productivity response of produced water.

Current hydrochemical research focuses on the chemical composition of groundwater, the sources of groundwater, spatiotemporal distribution patterns, water–rock interactions in different media, and the impact of hydrodynamic zoning on CBM enrichment (Rezaei et al. 2021; Huang et al. 2017; Tang et al. 2016; Sun et al. 2023). In terms of indicating CBM production, previous work has focused on conventional ion analysis (Shi et al. 2017; Du et al. 2020). There has been limited exploration of the hydrochemical information provided by trace elements and hydrogen and oxygen isotopes, reflecting a lack of deeper investigation into the characteristics of coal reservoirs and CBM production. In addition, engineering factors during the production process can lead to produced water being contaminated by fracturing fluids; a problem which is often overlooked (Sun et al. 2022; Qin et al. 2023). Consequently, a comprehensive analysis

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linking the full suite of hydrochemical indicators in produced water to CBM well productivity remains insufficient.

The Gujiao block in the Xishan coalfield is one of the key development blocks for CBM in China (Mo et al. 2012; Feng 2018). Currently, there are over 700 CBM wells drilled (Xia et al. 2019), with the majority already in production. However, there is a high proportion of low or non-producing wells (Xia 2017). Wang et al. (2018) have argued that groundwater with strong hydrodynamic conditions is unfavorable for the preservation of CBM (Wang et al. 2018). Zhu et al. (2018) and Zeng et al. (2019) found that the gas content in Gujiao block is closely related to the groundwater flow system and structure.

Currently, scholars have studied the produced water from CBM wells in areas with relatively simple geological structures such as Fanzhuang, Anze, Shizhuang, and Shouyang in the Qinshui Basin. They found that hydrochemical parameters are closely related to CBM accumulation and production (Wang 2023; Xu et al. 2016; Huang 2020). However, there has been relatively little analysis of the productivity response of produced water from the Gujiao block.

In this paper we examine the geochemical characteristics of produced water from the Gujiao block through conventional ions, trace elements, and isotopes. The study identifies indicators of fracturing fluid interference, explores the effects of ion composition on CBM productivity, and reveals the response mechanisms of geochemical characteristics to productivity. The aim is to support efficient CBM exploration and development in the region.

Geological background

The Xishan coalfield of Shanxi Province is located in the outer zone of the eastern wing of the “Qilvhelan” arc structure at the southern end of the east–west tectonic belt of Yangqu-Yuxian County (Fig. 1a). The southeast portion of the coalfield is connected to the Fenhe tectonic basin. The main tectonic framework is the development of north–south, east–west and north-east-east structures (Meng 2023; Yan et al. 2021). The Gujiao block is located in the middle of Xishan Coalfield. The main body is a monoclinic structure. The internal structure of the block composes mainly NE-SW structural elements which are controlled by faulting. The main orientation is 50°–70°. The fault structures are mostly tensile and torsional normal faults. Between the fault zones, on both sides of the fault plane, the fault structures are often accompanied by short-axis folds. Most of these fault zones show an echelon distribution (Fig. 1b).

The main coal-bearing strata in study area are the Shanxi formation of the lower Permian and the Taiyuan formation of the upper Carboniferous. The Shanxi formation is between 42 and 113 m thick (see the stratigraphic column in Fig. 1c). This formation is a set of coal-bearing rock series composed of sandstone, mudstone, coal seams, a small amount of marine shale, and laminated cone limestone, of which the 2# coal is a stable, mineable coal seam. The Taiyuan formation is between 49 and 126 m thick (Fig. 1c). The Taiyuan formation in the study area consists of mudstone, sandstone, siltstone, between 4 and 6 layers of limestone, and 6 to 8 layers of coal seams, with the 8th and 9th coal seams being the main coal seams for extraction.

There are three sets of aquifers developed in the study area. The CBM produced water mainly originates from the weak aquifers near coal seams, including Ordovician carbonate rocks, Carboniferous-Permian clastic rocks, and Quaternary loose sedimentary layers (Zhang 2014).

Samples and experiments

A total of 31 CBM well water samples were collected in the study area, with two bottles of water samples collected from each well. Sampling points were evenly distributed throughout the study area. Clean 500 ml polyethylene plastic

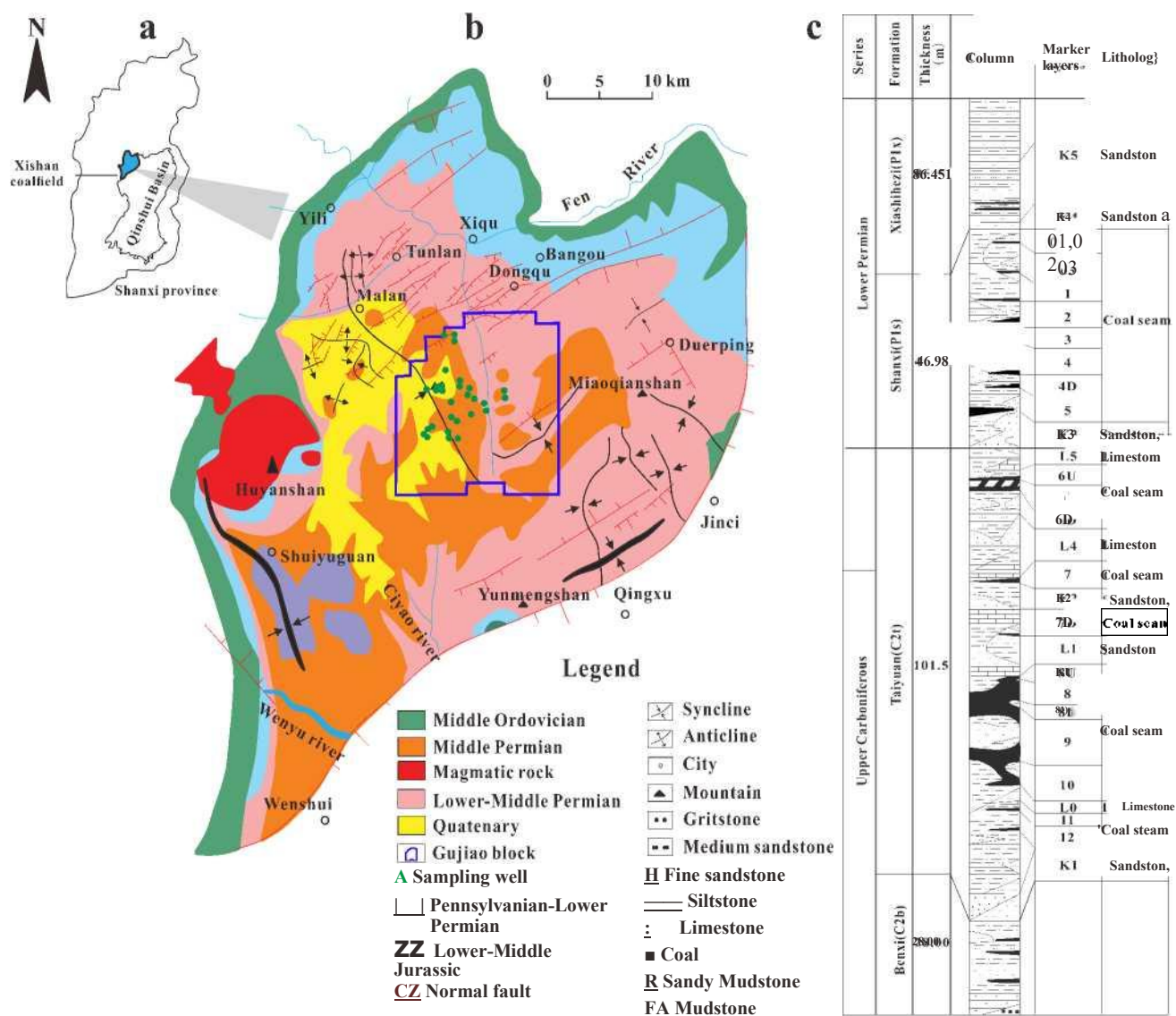


Fig. 1 Structural map and comprehensive stratigraphic column of the Xishan Coalfield and Gujiao block (Wang et al. 2018; Yan et al. 2021)

bottles were used to collect water samples. The bottles were rinsed with water samples three times to ensure there were no impurities inside the bottles before collecting the main sample. Water samples were collected directly from the CBM wellhead, ensuring to expel air from the bottle when sealing the cap to prevent changes in isotope content from long-term exposure to air. The bottle mouths were sealed with tin foil and the sample was wrapped with a black polyethylene bag. The samples were delivered immediately to the testing institution for analysis. Conventional ions, trace elements and isotopes were determined by inductively coupled plasma spectrometry, inductively coupled plasma mass spectrometry and stable isotope ratio mass spectrometry. All raw water test data are shown in Table 1.

Results and discussion

Geochemical characteristics of produced water from CBM wells

Conventional ion characteristics

According to the conventional ion test data of 31 CBM wells, the groundwater is mainly Cl-Na type, followed by HCO₃-Na type. Please see Table 1 for both values for individual wells as well as the arithmetic mean for each measurement.

The Total Dissolved Solids (TDS) of the produced water ranged from 1048 to 8610 mg/L, with an arithmetic mean of 2918.1mg/L. This range falls within the category of slightly

Table**1** Selected ion composition of produced water in CBM wells

Well	TDS	Conventional ions (mg/L)								
	(mg/L)	Ca ²⁺	K ⁺	Mg ²⁺	Na ⁺	HCO ₃ ⁻	CO3 ²⁻	Cl ⁻	SO4 ²⁻	Sr ²⁺
C-1	2228	7.7	64.5	3.5	884	419.1	12.4	1168.7	4.5	3700
C-2	2831	23.9	99.1	6.5	1080	587.7	10.9	1414.2	4.1	2250
C-3	1958	14.5	33.1	3.6	797	742.1	22.5	815.8	4.9	1790
C-4	2750	2.8	32.2	1.9	1180	1900.1	72.8	608.2	3.9	1270
C-5	2038	14	34.2	4.2	802	768.9	26.4	845.1	3.3	1700
C-6	2148	10.7	30.3	3.7	859	1192.7	44.9	603.3	3.3	918
X-1	2258	15.9	133	4.7	846	962.7	34.1	847.6	2.5	2460
X-2	3286	31.1	160	9.0	1190	734.2	31.0	1538.8	3.3	5490
X-3	1830	5.9	16.3	2.3	776	1161.2	54.2	517.8	4.1	1260
X-4	2234	16.3	16.5	3	913	1022.5	41.8	791.4	3.3	4000
X-5	2484	6.9	64.1	2.6	966	773.6	35.6	1024.6	4.9	2510
X-6	2548	1.3	36.2	1.2	1070	1326.6	80.6	774.3	3.7	888
X-7	5848	85	65.7	15.2	2060	82.7	12.4	3439.0	3.3	21200
X-8	1490	5.3	9.46	1.2	609	682.2	24.8	508.0	4.5	792
X-9	2186	2.4	40.1	1.9	878	743.7	52.7	862.2	4.1	1210
X-10	3880	12	46.8	4.0	1530	634.9	12.4	2007.7	2.9	4260
X-11	2344	3.9	43.7	1.5	979	1291.9	72.8	649.7	3.7	823
X-12	2708	12.2	37.7	5.2	1080	1274.6	72.8	901.3	2.5	2180
X-13	2632	8.3	33.6	2.8	1120	1021.0	40.3	1177.3	2.9	1880
X-14	2740	9.7	55.3	2.1	1120	1162.8	71.3	1106.5	4.9	6620
X-15	4001	6.4	28.1	4	1710	1425.9	77.5	1691.4	3.5	696
X-16	4332	16.1	149	5.1	1730	1163.5	44.2	2088.3	2.5	3420
X-17	2352	5.9	347	9.1	883	779.9	41.8	1023.4	9.1	747
X-18	2888	2.9	9.99	1.7	1240	1454.2	69.7	1013.6	2.9	445
X-19	1048	6.5	4.38	5.01	448	444.3	12.4	471.4	3.3	987
Z-1	8610	70.3	991	16.5	2580	1159.6	15.5	4567.5	2.5	4870
Z-2	1794	11.2	17.4	3.1	733	872.9	34.1	593.5	5.8	343
Z-3	2406	7.8	39.8	2.7	1020	1793.0	69.7	461.6	3.3	512
Z-4	2090	5.8	76.9	1.6	856	1455.8	43.4	469.0	3.3	480
Z-5	1848	4.3	36.1	1.9	761	1353.4	71.3	327.3	3.3	570
Z-6	6670	39.9	470	10.4	2220	1358.1	31.0	3280.3	3.3	2930
Mean	2918	15.1	104	4.6	1126	1024	43.1	1212.5	3.8	2684

Well	Trace elements (µg/L)						Isotopes		
	Ba ²⁺	Li ⁺	Mn ⁿⁿ⁺	Rb ⁺	Zn	Cs	Mo	δ18O	δ ² H
C-1	8570	218	65.3	39.1	12.5	2.2	26.9	-9.3	-62.8
C-2	2800	367	279	44.7	7.6	1.6	2.8		
C-3	2070	172	187	15.7	34.1	0.6	20.5		
C-4	1110	129	85	13	15.3	0.4	13.5		
C-5	1640	177	107	26.5	10.3	0.8	36		
C-6	1780	301	54.5	21.4	7.6	0.7	21.7		
X-1	3770	283	59.1	49.3	8.3	1.5	6.7		
X-2	7040	461	164	56.3	8.8	2.1	69.8		
X-3	1660	158	59.8	13.6	10.4	0.6	10.7	-9.7	-66.2
X-4	14,600	224	51.3	24.3	12.8	1.3	20.9		
X-5	9980	236	21.7	24.7	8.5	1.8	24		
X-6	2320	187	10.2	21.9	7.2	1.5	147		
X-7	25,000	195	399	34.6	11.4	1.3	25.1		
X-8	764	73.1	67.5	8.4	7.1	0.3	12.7		
X-9	4110	137	9.3	11.9	10.9	1.0	72.1		
X-10	6210	287	274	29	11.4	1.5	12.8		
X-11	1760	225	24.3	22	6.0	1.0	14.9	-9.1	-59.6
X-12	4450	193	51.6	28	7.9	1.2	11.4		
X-13	4270	213	28	29.8	5.6	1.3	5.3		
X-14	26,500	236	13.6	28.4	14.1	2.1	64	-3.9	-39.1

Table 1 (continued)

X-15	1500	147	34.8	20.1	6.4	1.1	14.5	-9.7	-66.9
X-16	1040	208	62.9	34.8	9.6	1.5	16.2		
X-17	1510	118	14.3	16.7	11.1	0.8	28.5		
X-18	1200	115	48.3	12.7	4.6	0.8	24.3		
X-19	2400	66.2	38.8	5.7	8.5	0.3	33.6	-5.8	-46.7
Z-1	9200	858	333	139	7.6	6.4	7.5		
Z-2	1600	149	5.9	16.2	4.8	0.7	12.7		
Z-3	2060	180	46.7	21.1	8.4	0.7	10.1		
Z-4	1970	114	60.6	24.1	8.4	0.6	2.8		
Z-5	1230	158	44.8	13.1	8.2	0.5	14.6	-9.6	-63.5
Z-6	6820	475	104	65.6	6.7	2.4	6.7		
Mean	5191	228	90.5	29.4	9.7	1.3	25.5	-8.3	-57.8

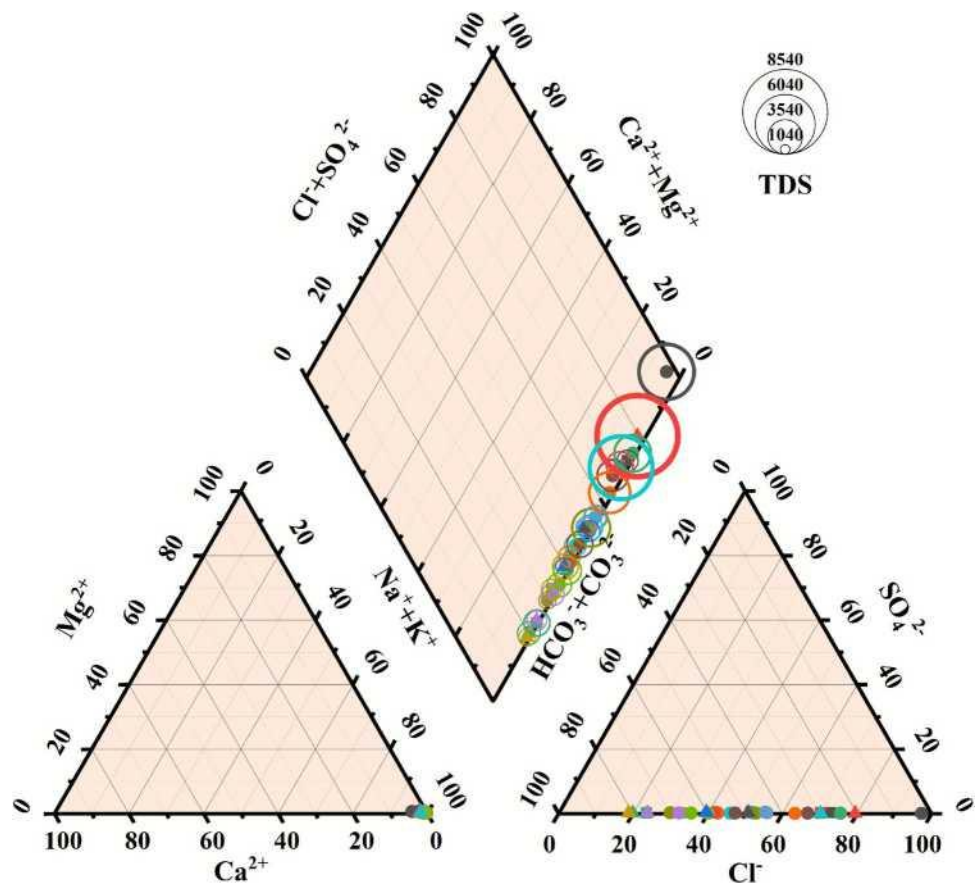
Mean Arithmetic mean over all values in the column

brackish to brackish water (Fig. 2). The main cation is Na^+ , with concentrations ranging from 448 to 2580 mg/L, with an arithmetic mean of 1123.45 mg/L, followed by K^+ , while Ca^{2+} and Mg^{2+} have very low. The main anion is Cl^- , with concentrations ranging from 327.3 to 4567.48 mg/L, with an arithmetic mean of 1212.55 mg/L, while HCO_3^- , SO_4^{2-} , and CO_3^{2-} contents are low.

A number of hydrochemical indices have been used to quantify the main ions in the groundwater. The $[\text{Na}^+]/[\text{Cl}^-]$ ratio is used to characterize the degree of enrichment of Na^+ in groundwater (Egbueri et al. 2021). Here, the square

brackets indicate the concentration of the ion as given in Table 1, but converted to meq/L. All but two of the samples have an $[\text{Na}^+]/[\text{Cl}^-]$ ratio greater than unity, indicating that the water has undergone silicate rock weathering, with Na^+ mainly derived from the dissolution of silicate rocks (Fig. 3a). Some samples have ratios below 1, indicating significant contamination by fracturing fluids.

Water–rock interactions also occur during groundwater flow, leading to ion exchange. The Chloro-Alkaline Index (CAI) is a geochemical parameter used to understand ion exchange processes between groundwater and

Fig. 2 Piper diagram of ground-water chemical types and ion concentrations

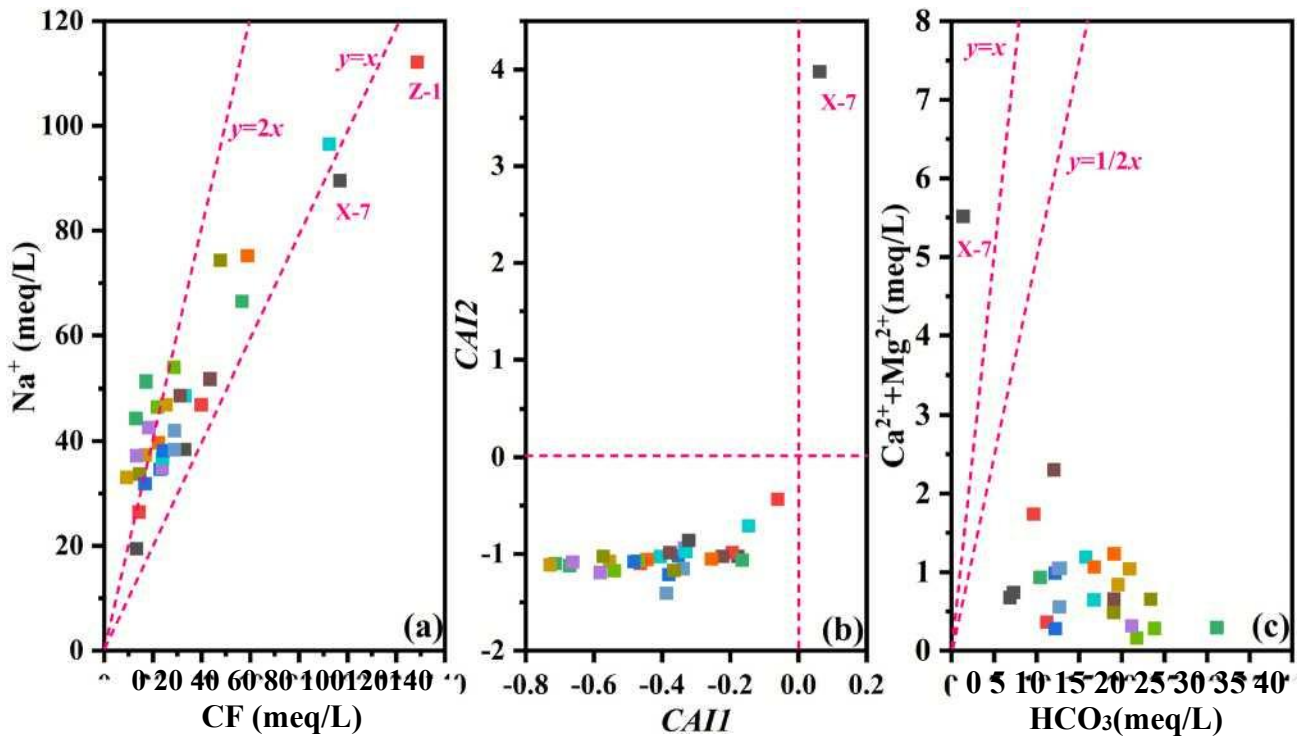


Fig. 3 Mineral dissolution equilibrium diagrams. **a** Na^+/Cl^- ; **b** Chloro-Alkaline Index (CAI); **c** $(\text{Ca}^{2+} + \text{Mg}^{2+})/\text{HCO}_3^-$

its surrounding rock environment. It helps in identifying interactions that occur as groundwater moves through different geological formations. There are two indices, CAI1 and CAI2 , which are calculated using the concentrations of chloride (Cl^-), sodium (Na^+), and potassium (K^+) ions in the water. The indices are given by

$$\text{CAI1} = \frac{[\text{Cl}^-] - ([\text{Na}^+] + [\text{K}^+])}{[\text{Cl}^-]} \quad (1)$$

and

$$\text{CAI2} = \frac{[\text{Cl}^-] - ([\text{Na}^+] + [\text{K}^+])}{[\text{HCO}_3^-] + [\text{CO}_3^{2-}]} \quad (2)$$

Positive values of CAI indicate that sodium and potassium ions have been exchanged with calcium and magnesium ions in the groundwater, while negative values suggest the opposite (Zhang et al. 2020). If CAI1 and CAI2 are both negative, there has been an exchange of cations between groundwater and surrounding rocks, where Ca^{2+} and Mg^{2+} are adsorbed by the matrix from the groundwater, and Na^+ and K^+ are released from the surrounding rocks to dissolve in the groundwater. The data in this work (Fig. 3b) is consistent with this scenario. Consequently, cation exchange also

contributes to the high Na^+ groundwater content. However, both CAI1 and CAI2 for well X-7 are positive, indicating a reverse cation exchange process occurring near this well.

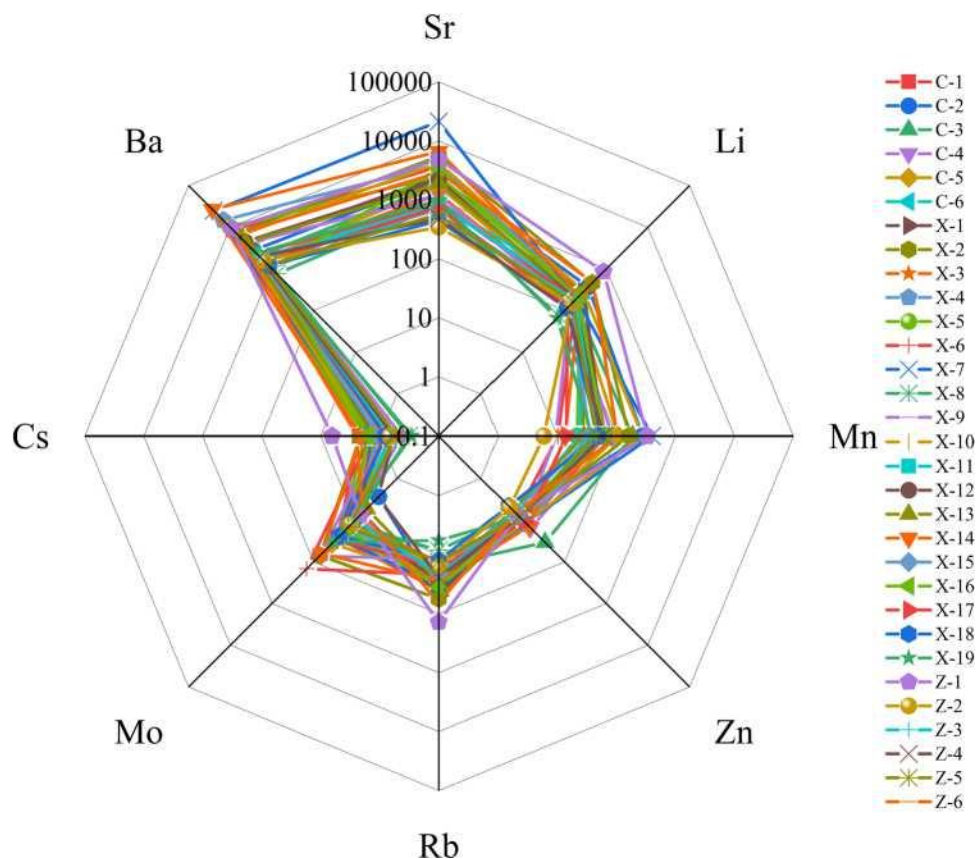
The $([\text{Ca}^{2+}] + [\text{Mg}^{2+}]) / [\text{HCO}_3^-]$ ratio can be used to determine the sources of Ca^{2+} and Mg^{2+} in groundwater (Maurya et al. 2019). The majority of groundwater samples have $([\text{Ca}^{2+}] + [\text{Mg}^{2+}]) / [\text{HCO}_3^-]$ ratios less than 1, except for X-7 (Fig. 3c), indicating that Ca^{2+} and Mg^{2+} mainly originate from the dissolution of carbonate rocks and silicate rocks. For well X-7, the high Cl^- content and reduced HCO_3^- concentration together indicate strong dissolution of developed aquifer evaporitic rock and/or possible contamination by fracturing fluid.

Trace element characteristics

Trace element analysis is an important method for studying hydrodynamic conditions and their origins. The trace element compositions measured in this work are shown in Fig. 4. Among the trace elements measured, Ba^{2+} and Sr^{2+} have the highest concentrations. The concentration of Ba^{2+} ranges from 764 to 26,500 $\mu\text{g/L}$, with an arithmetic mean of 5191.4 $\mu\text{g/L}$, and Sr^{2+} ranges from 343 to 21,200 $\mu\text{g/L}$, with an arithmetic mean of 2683.9 $\mu\text{g/L}$. The Cs^+ ion showed the lowest concentration in our data.

The Sr^{2+} content of continental aquifer water is known to be low, while high Sr^{2+} content often occurs in highly

Fig. 4 Radar chart of trace elements in produced water from CBM Wells



concentrated marine aquifer water or gypsum-salt rock formations (Ma et al. 2006). In our study area the groundwater exhibits high Sr^{2+} values, and there is a certain similarity in the enrichment of Ca^{2+} and Sr^{2+} (Fig. 5). From the perspective of ionic radii, Sr^{2+} has the same hydrated ionic radius as Ca^{2+} to 2 decimal places ($\text{Sr}^{2+} = 2.70\text{\AA}$, $\text{Ca}^{2+} = 2.30\text{\AA}$), and similar unhydrated ionic radius ($\text{Sr}^{2+} = 1.18\text{\AA}$, $\text{Ca}^{2+} = 1.00\text{\AA}$, both for the 2+ charge). During carbonate rock formation, CaCO_3 readily captures Sr^{2+} . The synchronous enrichment of Ca^{2+} and Sr^{2+} indicates they are released from dissolved calcium-containing minerals during water-rock interactions, suggesting that Sr^{2+} in the aquifer water mainly comes from the dissolution of minerals like plagioclase or cementitious calcite (Qin et al. 2011).

The combination of trace elements Ba^{2+} and Sr^{2+} often reflects the hydrogeological environment of marine and continental conditions. The higher concentration of Ba^{2+} ions also indicate a good reducing environment in the block (Li et al. 2008). The Ba^{2+} element content in the block is much higher than that in open sea water ($100\text{ }\mu\text{g/L}$), and some samples exceed the Ba^{2+} content in gulf sediments ($13,000\text{ }\mu\text{g/L}$), such as X-4, X-7, and X-14. Previous studies (Sun 2016) have found that the Shanxi formation, in the Gujiao block location, was formed in a deltaic environment, while the Taiyuan formation was formed in barrier

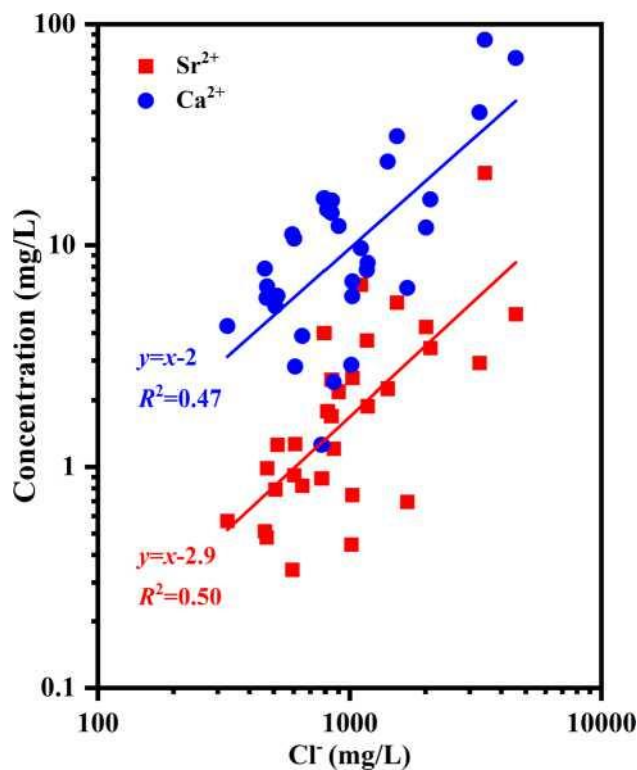


Fig. 5 Correlation between Cl^- , Sr^{2+} , and Ca^{2+} content in aquifer water

sandbars, swamps, and sediments forming in tidal flats. The high barium content in the aquifer water samples may be influenced by the sedimentation of the Taiyuan formation transitional phase between sea and land, resulting in a relatively high Ba^{2+} content.

Hydrogen and oxygen isotope characteristics

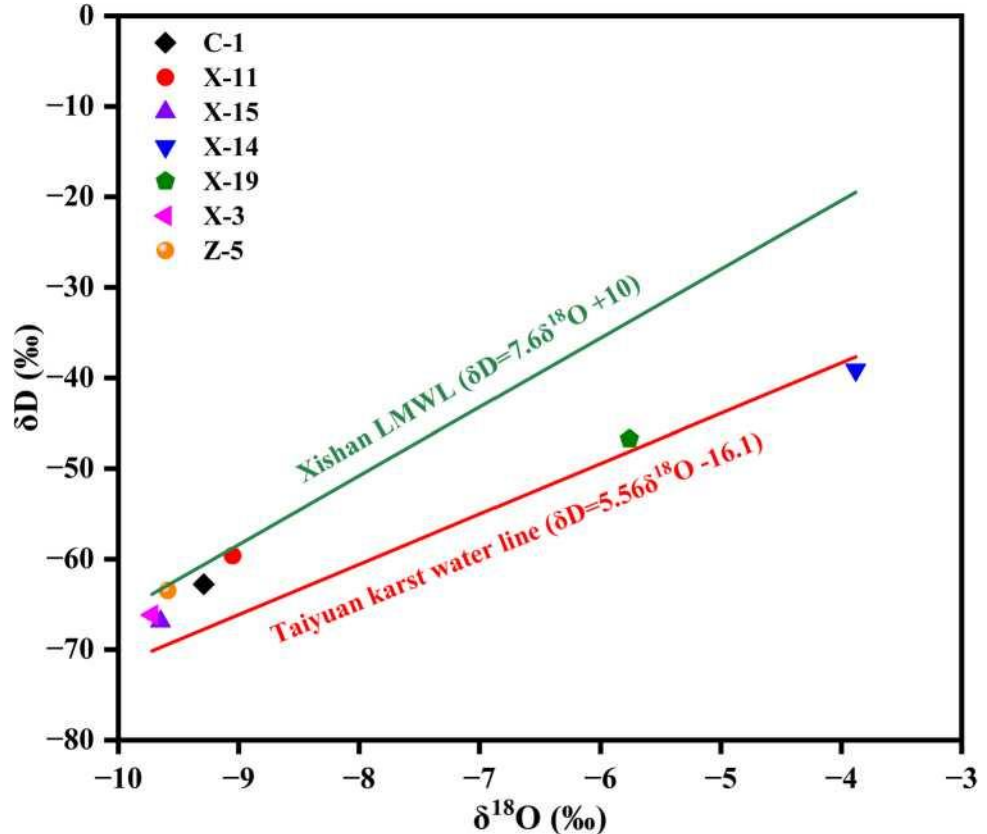
Hydrogen and oxygen stable isotopes can reflect the geochemical processes of groundwater and are important indicators for studying the hydrological cycle and dynamic characteristics of the groundwater. In this study, hydrogen and oxygen stable isotope tests were conducted on seven groundwater samples. The $\delta^{18}O$ values ranged from -9.72‰ to -3.88‰, with an arithmetic mean of -8.13‰, while the δD values ranged from -66.86‰ to -39.12‰, with an arithmetic mean of -57.82‰. The deuterium excess parameter, d , reflects the degree of exchange of δD isotopes in the region, and is not significantly affected by environmental factors such as latitude and seasonal conditions. The magnitude of d is equivalent to the intercept when the slope of the Local Meteoric Water Line (LMWL) $\Delta\delta D/\Delta\delta^{18}O$ is the value 8, i.e., $d = \delta D - 8 \times \delta^{18}O$ (Dansgaard 1964). The d values ranged from -8.08 to 13.24. Except for samples X-14 and X-19, which had negative d values, all other production layers

had positive d values. This indicates slow water circulation, facilitating oxygen isotope exchange and resulting in larger d values. By contrast, aquifer water replenished by precipitation has faster circulation, reducing oxygen isotope exchange and resulting in smaller d values (Liu et al. 2016).

The LMWL in the Xishan area is represented by $\delta D = 7.6 \times \delta^{18}O + 10$, while the karst water line in the Taiyuan area is represented by $\delta D = 5.56 \times \delta^{18}O - 16.1$ (Qian and Guo 2002; Wang and Xu 1993). The coal seam contains a complex mixture of hydrocarbons. If precipitation recharges coalbed water, the produced water from CBM wells will show deuterium drift, with isotopic composition above the LMWL. Conversely, sandstone and limestone waters show oxygen drift, with isotopic compositions below the LMWL.

The $\delta^{18}O$ values of groundwater samples in study area are all below the LMWL of the Xishan area (Fig. 6), indicating that the initial source of groundwater in study area is atmospheric precipitation. Apart from sample X-14, the isotopic compositions of the remaining samples fall between the LMWL of the Xishan area and the karst water line of the Taiyuan area, indicating that the produced water from CBM wells in study area mainly originates from sandstone water.

Fig. 6 Distribution relationship of hydrogen and oxygen isotopes in produced water from CBM wells



Mixed source and horizon identification of produced water in CBM wells

Hydraulic fracturing and other reservoir modification techniques are often used in CBM development due to the low permeability of coal seams. Consequently, the quality of produced water can be influenced by fracturing fluids remaining in the formation for a certain period.

It is necessary to exclude sample data contaminated by fracturing fluids in order to assess accurately the impact of produced water on CBM well productivity. This can be done on the basis of understanding the geochemical characteristics of produced water from CBM wells. This study, conducted on the SPSS platform, employed Q-type cluster analysis and Principal Component Analysis (PCA) on Z-score standardized hydrochemical data. The aim is to differentiate between coalbed water and contaminated water based on the variations and composition characteristics of ions in the produced water from CBM wells.

Q-type cluster analysis

Q-type cluster analysis is conducted by selecting parameters such as K^+ , Na^+ , Ca^{2+} , Mg^{2+} , SO_4^{2-} , Cl^- , HCO_3^- , and CO_3^{2-} as variables for clustering. In Q-type cluster analysis, an original matrix is established based on the sample test data, followed by normalization to eliminate the adverse effects caused by abnormal sample data variations. The Ward method is used to cluster the data, and the squared Euclidean distance was employed to measure distances between clusters.

The 31 water samples are divided into 4 clusters using a distance threshold of 4.8. Cluster C2 includes 18 samples, while clusters C1, C3, and C4 each include 9, 1, and 3 samples, respectively (Fig. 7). All four clusters show high concentrations of Na^+ and K^+ , along with elevated Cl^- , and relatively high concentrations of HCO_3^- and CO_3^{2-} , while other ion concentrations are low. Cluster C4, especially, displays exceptionally high Na^+ and K^+ concentrations, as well as Cl^- , with lower HCO_3^- and CO_3^{2-} concentrations. The cluster analysis simply clusters wells with similar data, and does not, in itself, indicate contamination. Wells Z-1, Z-6, and X-7 in the cluster C4 may have been contaminated by fracturing fluids, showing extremely high Cl^- characteristics. To assess the validity of the clustering outcome, a silhouette coefficient (SC) analysis is conducted for the four identified clusters. The results demonstrate a discernible cluster structure within the dataset, albeit with varying quality across clusters: C1 ($n = 9$, $SC = 0.60$) and C2 ($n = 18$, $SC = 0.54$) show reasonable structure, while C4 ($n = 3$, $SC = 0.45$) is weaker. C3 ($n = 1$, $SC = 1.00$) represents a singular point. Overall, the clustering solution is deemed reasonable.

Principal Component Analysis (PCA)

Principal Component Analysis is used to perform dimensionality reduction on the original data (Rezaei et al. 2021). Measurables with eigenvalues greater than unity were selected as principal components (PC), and the variance contribution rate was used as the weight of comprehensive scores to evaluate the variability of data within data clusters. The weight of each original parameter in the PC is represented by component loadings, which are used to calculate the PC scores of observed samples under a given PC.

The PCA was conducted on the 31 samples. According to the Kaiser criterion and Scree plot, two principal components, PC1 and PC2, with eigenvalues greater than 1 were selected, accounting for 55.79% and 78.86% of the variability in the dataset, respectively (Table 2). The PC1 value is characterized by strong positive loadings for K^+ , Na^+ , Ca^{2+} , Mg^{2+} , and Cl^- , with CO_3^{2-} having strong negative loadings (Fig. 8). The PC2 value is characterized by strong positive loadings for Na^+ , HCO_3^- , and CO_3^{2-} , with SO_4^{2-} having strong negative loadings. The PC1 represents the characteristics of a mixture of coalbed water and fracturing fluid, while PC2 exhibits the characteristics of original coalbed water (Tang et al. 2016). Consequently, it is clear that further interpretation of the compositions of water samples in the study area need to be conducted by analyzing them together with the clustering results and the results from PCA analysis. This interpretation is given in the following sub-sections.

Source of water produced by CBM

The results of PCA indicate that PC1 explains its influence on groundwater composition based on high concentrations of K^+ , Na^+ , Ca^{2+} , Mg^{2+} , and Cl^- . The sodium ion is a common and abundant ion in groundwater, lacking in discriminative significance. Generally, surrounding rocks have a stronger adsorption effect on K^+ , Ca^{2+} , and Mg^{2+} than Na^+ , resulting in lower concentrations of K^+ , Ca^{2+} , and Mg^{2+} in original groundwater.

The chloride ion is the main anion in fracturing fluids (Bai and Wu 2016), with stable properties and limited interactions with rocks, possessing a strong migration capability. When fracturing fluids are injected, the concentrations of these four ions increase abruptly even though Ca^{2+} , Mg^{2+} and Na^+ are not appreciably present in the fracking fluid. On one hand, the injection of fracturing fluids alters the original hydrodynamic environment, thereby inducing cation exchange and mineral dissolution—a process that has been substantiated in preceding sections. On the other hand, a portion of Cl^- originates from organic-bound chlorine complexes in coal. When chlorine forms such organic

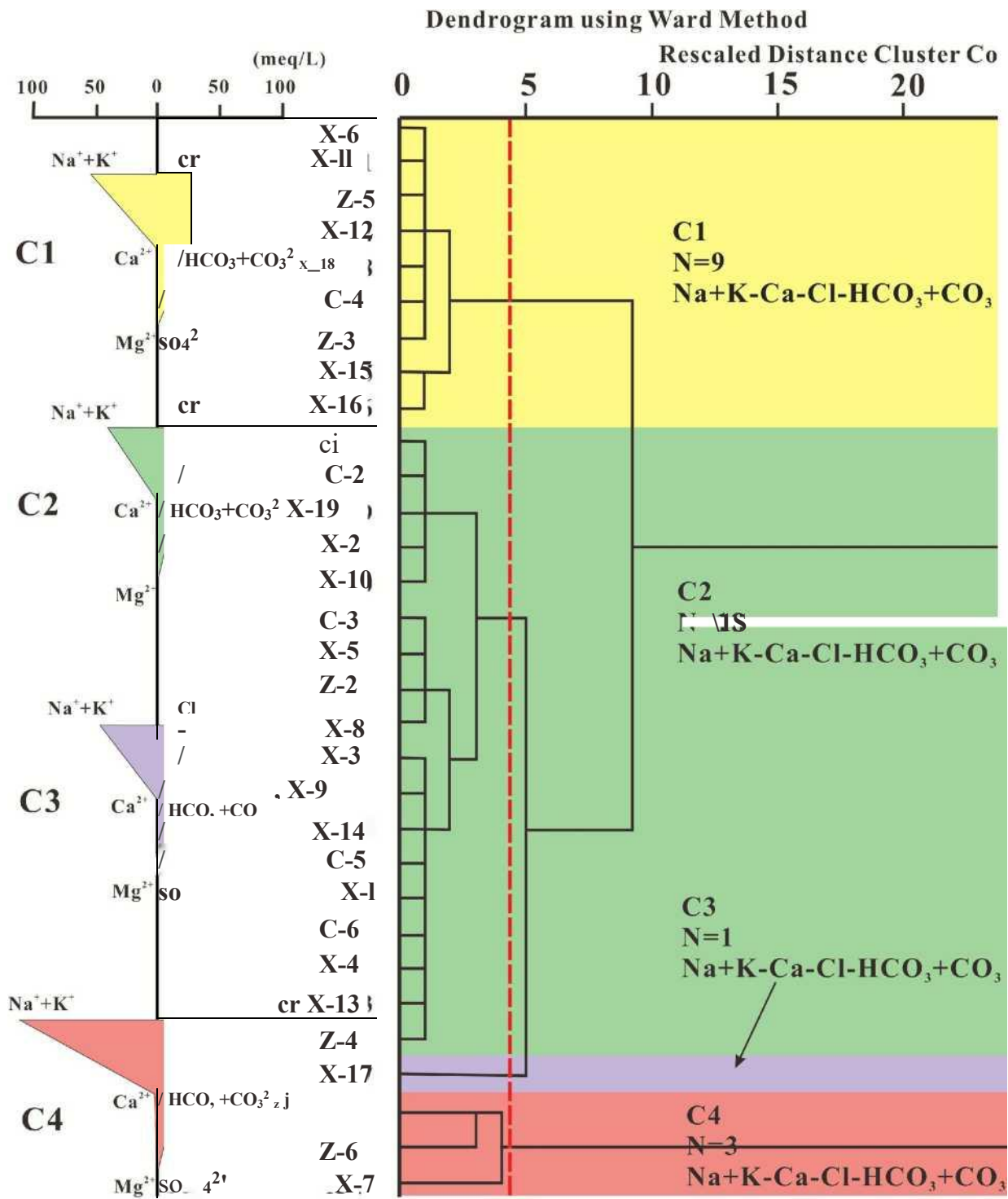


Fig. 7 Cluster pedigree diagram of CBM well water sample system

Table 2 Eigenvalues, variance, and component loadings of PC

Component	Eigenvalue	Variance	Cumulative variance	Loadings							
				Ca ²⁺	K ⁺	Mg ²⁺	Na ⁺	HCO ₃ ⁻	CO ₃ ²⁻	Cl ⁻	SO ₄ ²⁻
PC1	4.46	55.79	55.79	0.93	0.79	0.95	0.84	-0.31	-0.54	0.97	-0.21
PC2	1.85	23.07	78.86	-0.04	0.21	-0.08	0.44	0.90	0.73	0.15	-0.50

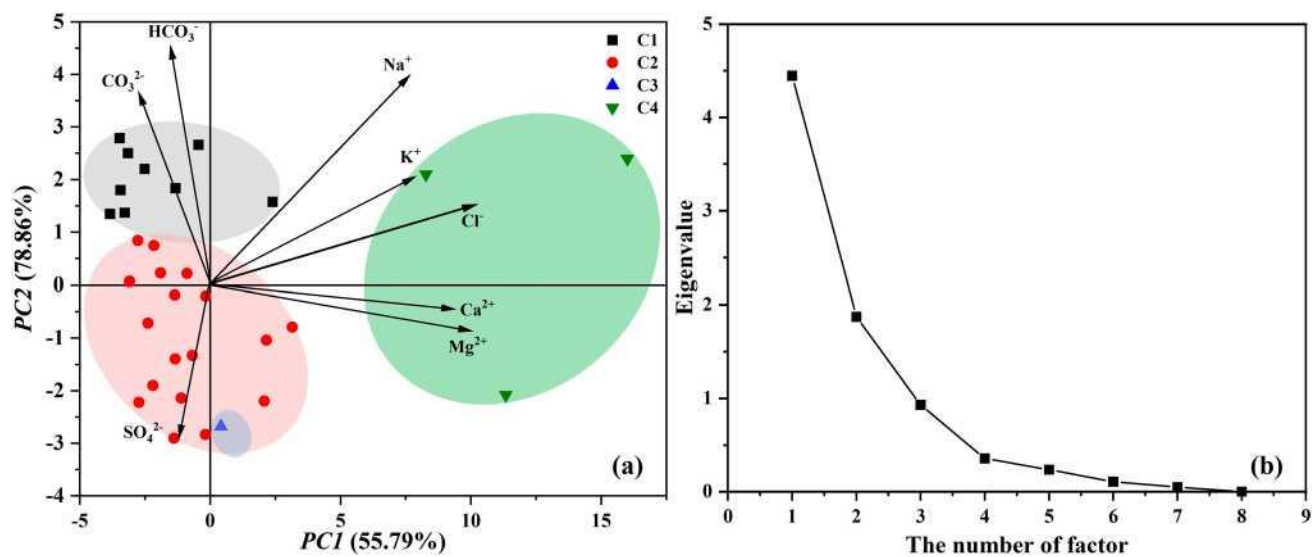


Fig. 8 The PC scores plot of water samples from the 4 clusters (a) and Scree Plot (b)

complexes in coal, it can associate with alkaline metal cations (e.g., Ca^{2+} , K^+ , Mg^{2+} , Na^+) by binding to polar oxygen groups in carboxylates or phenolates (Huggins and Huffman 1995). The release of chlorine from these organic-bound complexes is accompanied by the simultaneous release of associated alkaline metal cations (Yudovich and Ketris 2006). Therefore, with the release of Cl^- , the concentrations of Na^+ , Ca^{2+} , and Mg^{2+} increase. This study uses the concentrations of K^+ , Ca^{2+} , Mg^{2+} , and Cl^- as threshold indicators to assess the influence of fracturing fluids.

When the Cl^- concentration is below 60 meq/L, and the sum of K^+ , Ca^{2+} , and Mg^{2+} concentrations is below 2.5 meq/L, the K^+ , Ca^{2+} , and Mg^{2+} concentrations in samples from cluster C1 remain relatively stable as the Cl^- concentration increases (Fig. 9). However, samples from clusters C4, C3, as well as some from clusters C1 and C2, exhibit an increasing trend in K^+ , Ca^{2+} , and Mg^{2+} concentrations with increasing Cl^- concentration, which aligns well with the results of principal component analysis scores. It is concluded that in the study area, CBM well-produced water with Cl^- concentrations below 70 meq/L and K^+ , Ca^{2+} , Mg^{2+} concentrations below 2.5 meq/L can be considered unaffected by fracturing fluids.

Identification of water source layers

The main coal seams being mined in the study area are the 8# and 9# coal seams. This study primarily investigates the sources of formation water produced near the No. 8 and 9# coal seams. The Ordovician limestone has weak to moderate water saturation and is far away from coal seam, thus having minimal impact on CBM development in this area

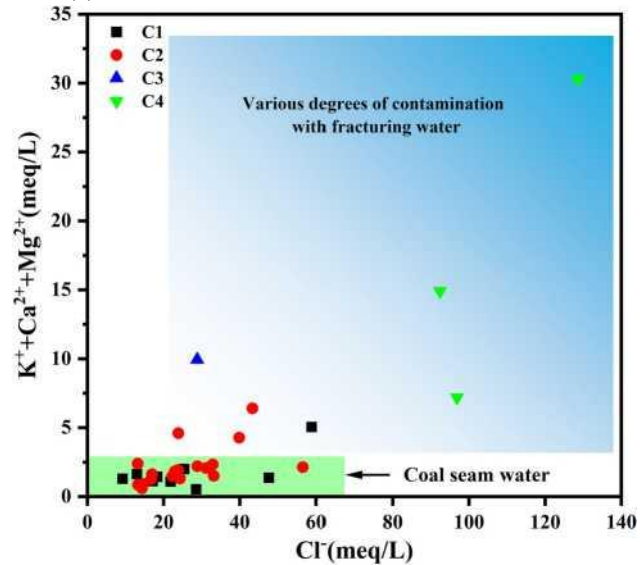


Fig. 9 Plot of the Cl^- versus $\text{Ca}^{2+} + \text{Mg}^{2+}$ relationship. The blue arrows indicate the direction of progressively greater contamination of the groundwater with fracturing fluids

(Li 2010). The main aquifers affecting CBM development in the study area include the sandstones of the Taiyuan formation. According to the stratigraphic classification standards of Shanxi Province, the Taiyuan Formation can be divided into: Member 1 (Dongdayao Member), Member 2 (Mao'ergou Member), and Member 3 (Jinci Member).

Using Archie's formula, 20 wells with complete data were analyzed to determine the water saturation and thickness of sandstone reservoirs in each coal-bearing stratum (Fig. 10).

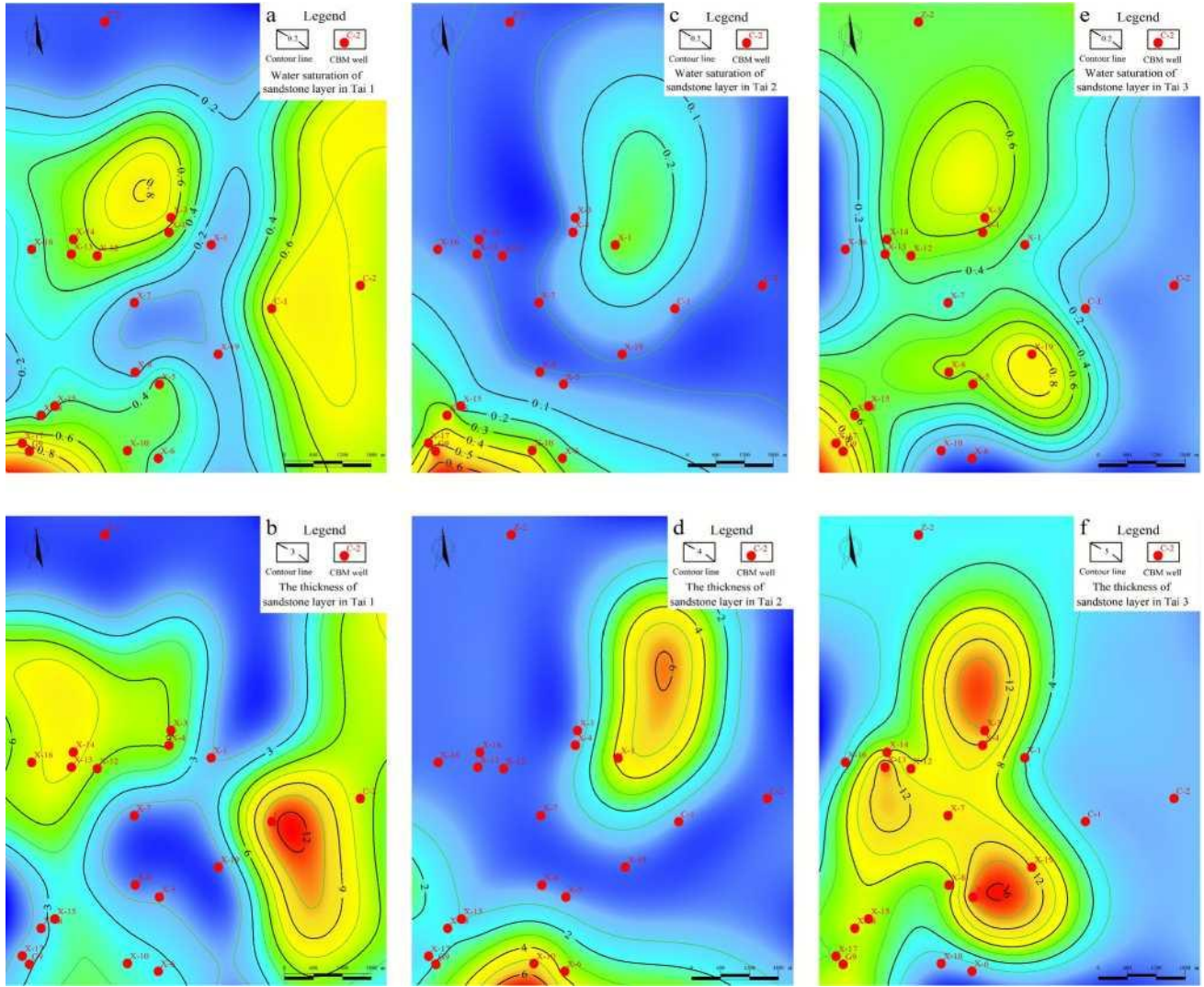


Fig. 10 The contour map of the thickness and water saturation of sandstone layers in different sections. **a** Water saturation in Member 1, **b** thickness of Member 1, **c** water saturation in Member 2, **d** thickness of Member 2, **e** water saturation in Member 3, (**f**) thickness of Member 3

$$S_w = \phi \frac{a b}{m-R} \frac{W}{R_t} \quad (3)$$

$$C = 1.698 * T - 62.98 \quad (4)$$

$$C = 2817.08 R_w^{0.78} \quad (5)$$

where, R_t is the deep investigation resistivity; R_w is the formation water resistivity, calculated using an empirical formula established in previous studies of this block (Zhao 2018); T is the measured salinity; C is the equivalent NaCl salinity; a and b are lithology coefficients; m and n is the porosity exponent and saturation exponent, respectively; ϕ is the porosity.

It is worth noting that the northern part of the block in Fig. 10 is not accurate enough, because the northern part is only controlled by single well factors. The sandstone

reservoir in Member 2 exhibits poor prospectivity, with low water saturation and thickness, indicating poor water-bearing properties. The sandstone reservoir in Member 3 shows high water saturation, maximum thickness, widest distribution, and closest proximity to the 8# and 9# coal seams in the vertical direction. Therefore, it is believed that the main source of water for the CBM wells in study area comes from the sandstone reservoir in Member 3.

Hydrochemical response of CBM productivity

The interaction between underground coal, gas, and water results from geological evolution. Thus, the geochemical characteristics of water from CBM wells can reflect the enrichment, migration, and production characteristics of CBM.

CBM well productivity characteristics

CBM well productivity varies significantly across the study area. Gas production data was collected from 132 wells. The arithmetic mean daily gas production for these 132 wells ranges from 54.4 to 3577.3 m³/d, with an arithmetic mean of 753.0 m³/d. About 80% of wells produce less than 1102.2 m³/d. Using the classification scheme by previous researchers (Guo et al. 2018), and the productivity characteristics of the Gujiao block, wells were categorized into as either high or low-to-medium gas rate wells based on the 80th percentile of average gas production rounded up to 1100 m³/d. Wells with a mean gas production above 1100 m³/d were classified as high gas rate wells, while those below 1100 m³/d were low-medium gas rate wells. The hydrodynamic and ion response characteristics of high and low-medium gas rate wells were analyzed and discussed separately based on sampling data (Fig. 11).

The control action of the hydrodynamic field

The CBM wells will form a pressure drop funnel at the wellhead during the initial production, and the water level of underground water will continue to decrease. This study selected CBM wells that have been in production for more than one year and calculated statistically the equipotential water level at the same date to more accurately reflect the characteristics of the coal seam groundwater flow field.

The water table elevation in the study area ranges from -12.2 to 677.0 m, indicating groundwater flows from northeast to southwest. The 340 m and 540 m contour lines (blue contours in Fig. 12a) are selected as boundaries for

hydrodynamic zoning. The northeast is the runoff area, the central part is the weak runoff area, and the southwest is the stagnation area (Fig. 12a). The box plot shows TDS ranges from 1048 to 3286 mg/L in the runoff area and from 1794 to 8610 mg/L in the stagnation area. Weaker runoff conditions correlate with higher TDS (Fig. 12b).

High gas rate wells are mostly horizontal wells and located near strong hydraulic gradients. They transition from the runoff area to the weak runoff area, and the gas production from horizontal wells increases significantly. Low and medium gas rate wells are characterized by vertical wells and are mostly distributed in the weak runoff and stagnation areas. Except for wells like X-8 and X-9, which were affected by construction and unable to produce adsorbed gas normally. For these wells, gas production remains low despite being in weak hydraulic areas. Analyzing wells separately shows a weak negative correlation between CBM gas production and groundwater table (Fig. 12c). Gas production is higher in weak hydraulic areas than in strong ones.

Response identification of CBM well productivity based on hydrochemical index

This study mainly analyzes the productivity of gas wells from the perspective of conventional ions, trace elements, and hydrogen and oxygen isotopes. The analysis reveals significant differences in the response of different hydrochemical indicators to production capacity between high-yield and low-yield wells (Fig. 13). Among them, Sr²⁺, Ba²⁺, and isotopic analysis are mainly based on joint analysis of high gas rate and low and medium gas rate wells, with

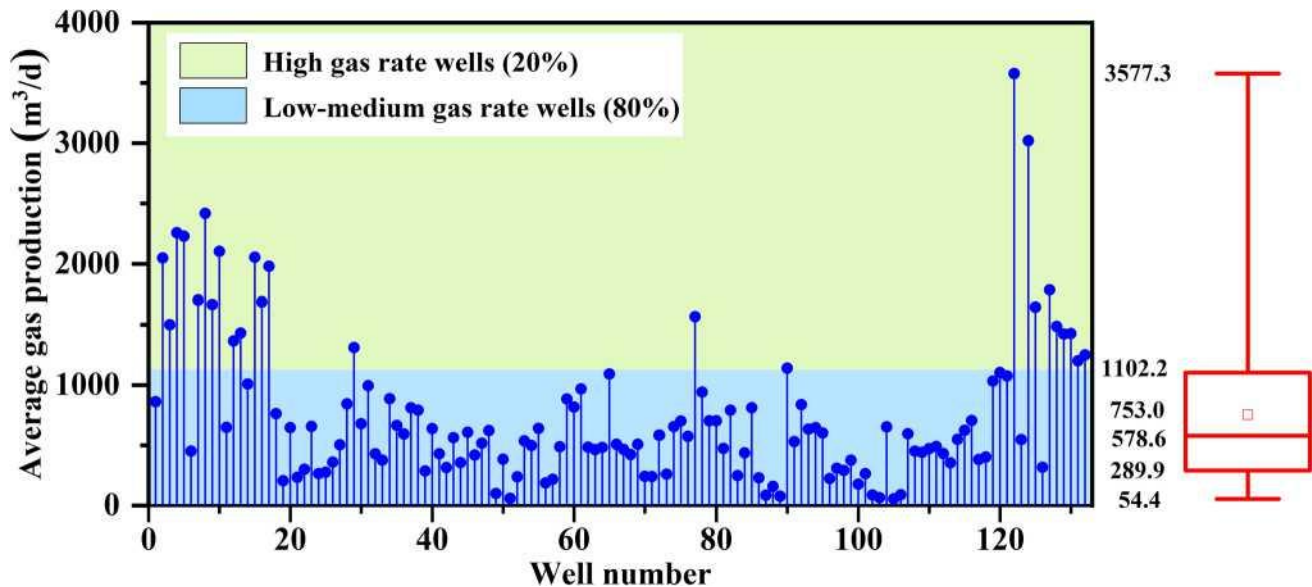
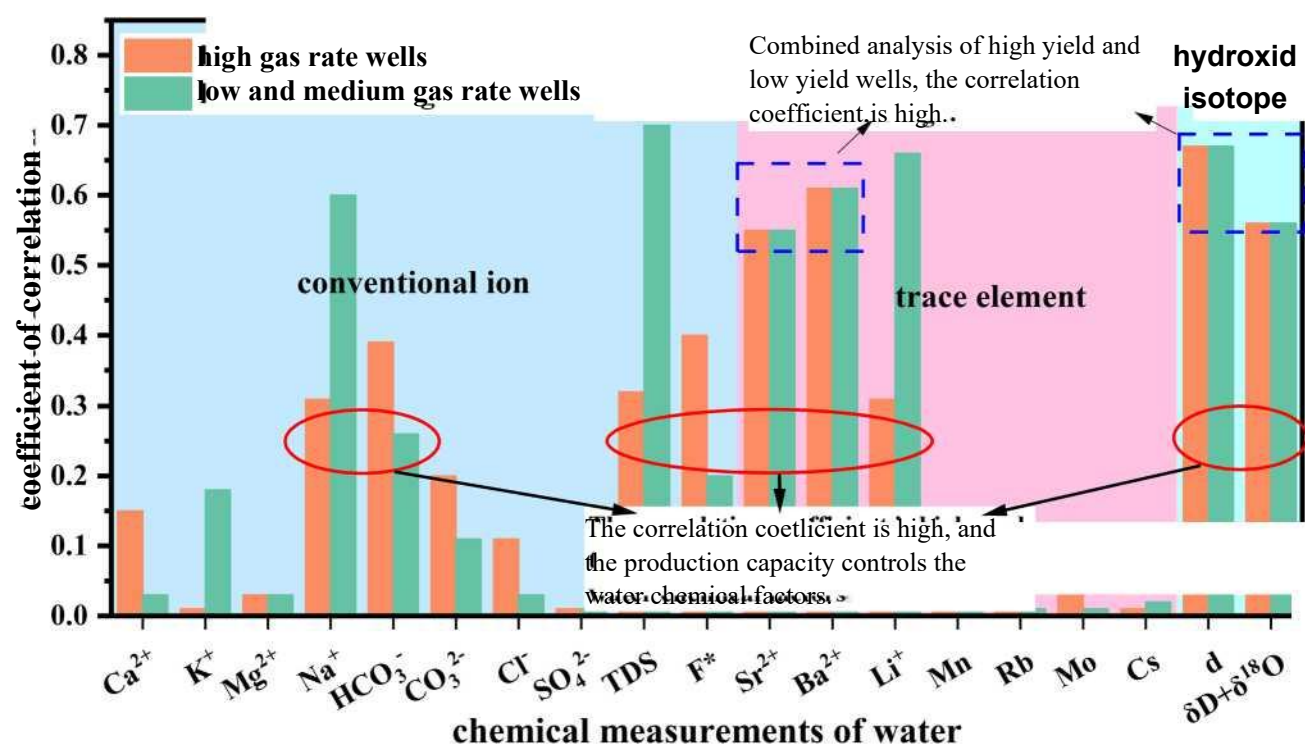
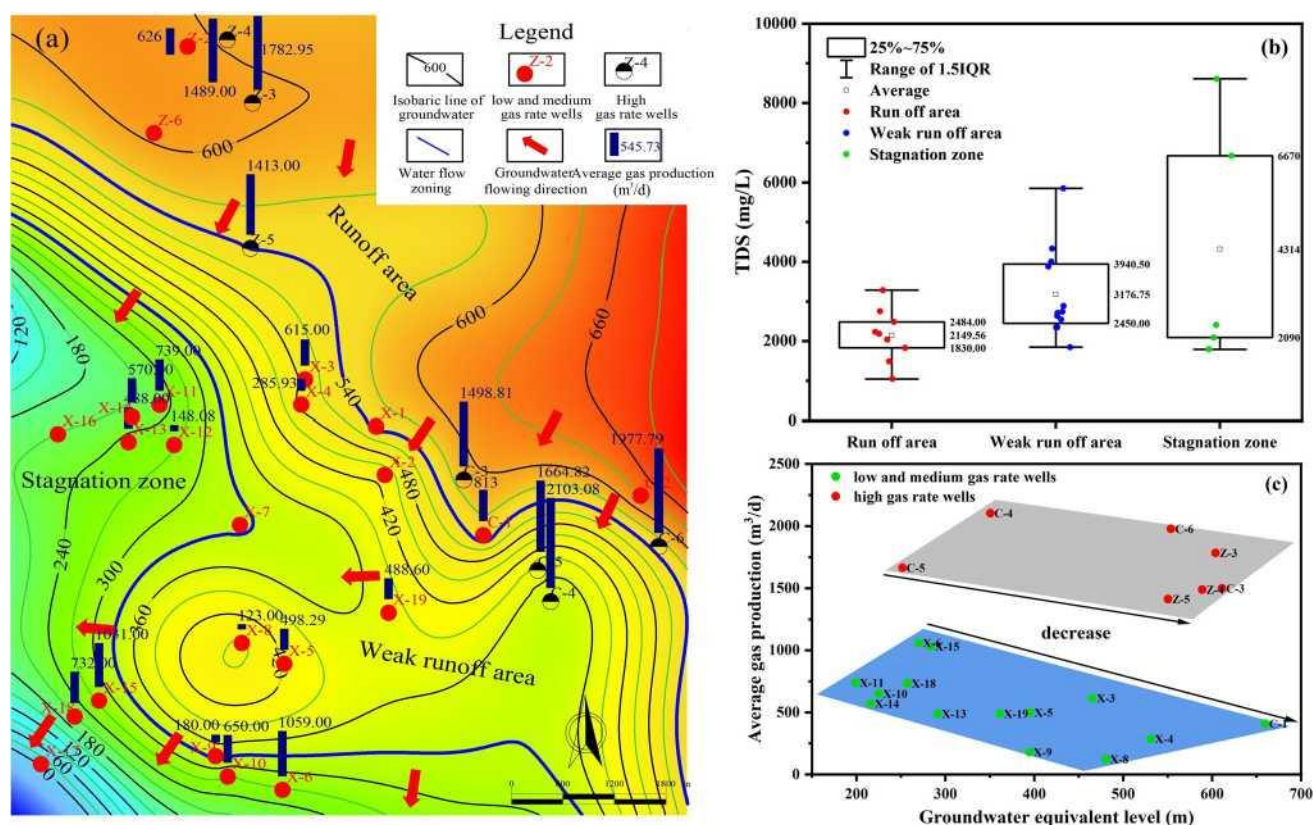


Fig. 11 Production capacity and classification criteria of CBM wells



high correlation coefficients. Overall, Na^+ , HCO_3^- , TDS, Sr^{2+} , Ba^{2+} , Li^+ , d -value, and $\delta\text{D} + \delta^{18}\text{O}$ show good correlation. The discussion will now focus on these hydrochemical parameters.

The response of conventional ions to production capacity

Analyzing 23 wells after removing the influence of hydraulic fracturing, it was observed that, unsurprisingly, high gas rate wells are all horizontal wells, while low and medium gas rate wells are all vertical wells. Therefore, the two are discussed separately.

From the correlation of hydrochemical indicators (Fig. 14), it can be seen that in both high and low-medium gas rate wells, TDS and Na^+ are positively correlated with gas production. Here, only the influence of TDS is analyzed, especially the strong correlation in high gas rate wells. Due to the disruptive effect of groundwater flow on the enrichment of CBM reservoirs, under the same mining conditions, the high mineralization and high sodium ion characteristics in locally stagnant groundwater areas are conducive to the

enrichment and production of CBM, which is consistent with the hydraulic control effect mentioned earlier.

The concentration of HCO_3^- in produced water is positively correlated with the daily average gas production. During dewatering and depressurization, CO_2 solubility produces high HCO_3^- concentrations in wells with more gas production. Additionally, sulfate ion reduction in groundwater flow increases HCO_3^- while decreasing SO_4^{2-} . Generally, in an open hydrological environment close to the oxygen-rich water recharge area, Ca^{2+} and Mg^{2+} are relatively enriched, while in a closed groundwater environment far from the water recharge area, Na^+ , Cl^- , and HCO_3^- are relatively enriched. Therefore, we introduce a groundwater closure index (F^*) to evaluate the degree of groundwater environmental closure from the perspective of ion composition. In this block, however, the presence of produced water contaminated by fracturing fluid obscures the original formation water information, and the fracturing fluid resists rapid flowback. Accordingly, we modify this index by incorporating previous research findings (Wu et al. 2018; Chen 2015; Wu 2019), with the specific expression given as follows:

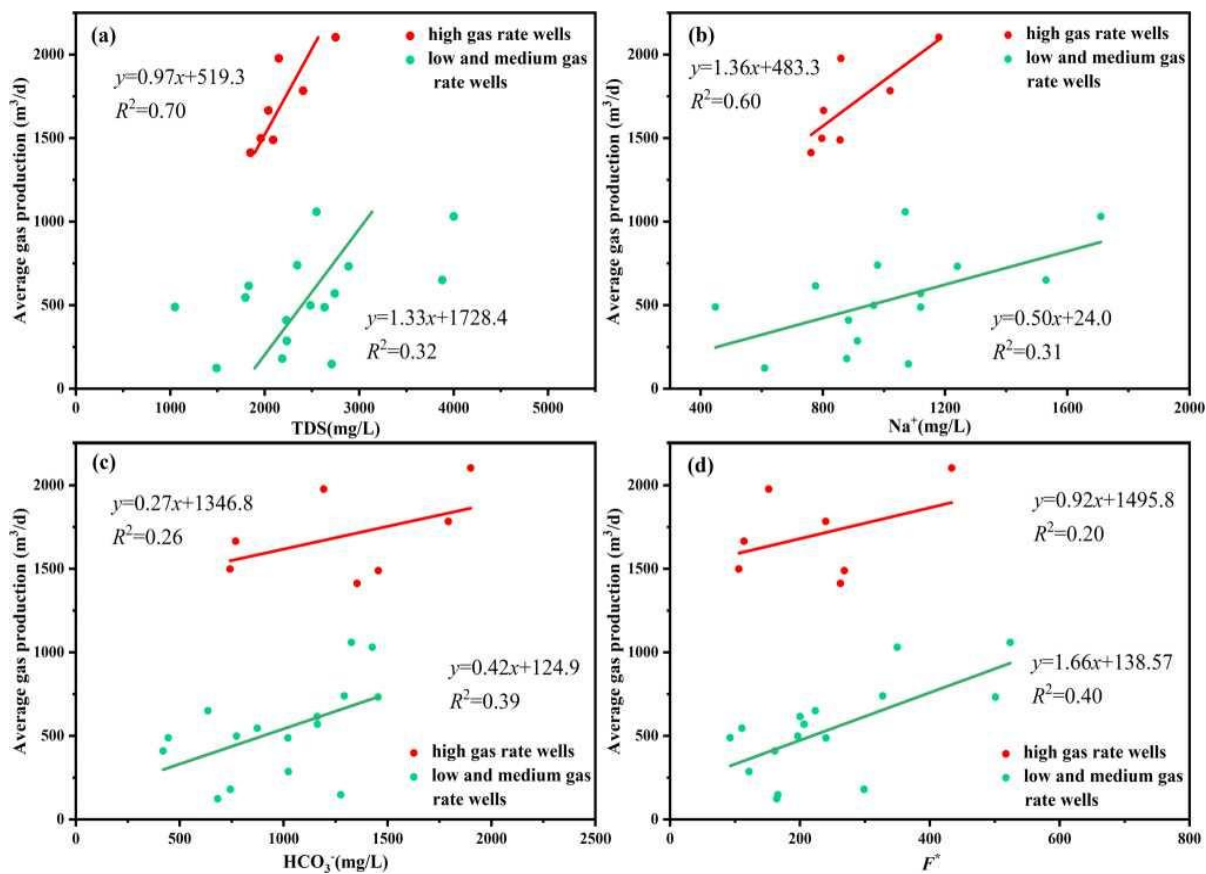


Fig. 14 The relationships between daily gas production rate and **a** TDS, **b** Na^+ , **c** HCO_3^- , and **d** F^* in high and low gas rate wells

$$F^* = \frac{[K^+] + [Na^+] + [HCO_3^-] + [CO_3^{2-}] + [Cl^-]}{[Ca^{2+}] + [Mg^{2+}] + [SO_4^{2-}]} \quad (6)$$

where the square brackets represent the mass concentrations of each ion in mg/L, and F^* is consequently dimensionless.

The F^* of underground water ranges from 92.44 to 524.03, with an arithmetic mean of 237.41. As F^* increases, the daily gas production gradually increases. With F^* less than 700, the underground water closure is relatively weak, and the hydrodynamic conditions are active, which is conducive to the drainage and depressurization of CBM wells, resulting in continuously increasing daily gas production (Chen 2015).

Conventional ions like TDS, HCO_3^- , and F^* show a significant positive correlation with gas production, serving as geochemical characteristics for evaluating production potential, making them useful for evaluating production potential.

The response of trace elements to production capacity

The relationship between the concentration of trace elements in coalbed water and gas production has also been investigated. The results showed that the concentration of lithium was positively correlated with daily gas production, and the correlation was higher in high gas rate wells (Fig. 15). The Li^+ concentration showed a certain association with HCO_3^- ,

indicating a certain affinity for bicarbonate ions (Nian et al. 2019). The concentrations of Sr^{2+} and Ba^{2+} elements were significantly negatively correlated with daily gas production, and the two elements showed similar behavior. This may be related to their similar chemical properties. High gas rate wells exhibited low Sr^{2+} and Ba^{2+} concentrations. Both Sr^{2+} and Ba^{2+} belong to alkaline earth metals, and during the migration process in water, Ba^{2+} tends to precipitate first as $SrSO_4$, leaving Sr^{2+} relatively enriched in the water. When the salinity of the water increases, Sr also increases in the form of $SrSO_4$ precipitation. The enrichment patterns of Ca^{2+} and Sr^{2+} in formation water exhibit similarities, indicating that the precipitation of $SrSO_4$, $BaSO_4$, and $CaSO_4$ can block the small pores in coal seams (Nian et al. 2019), limiting the production efficiency of CBM. Current experimental studies indicate that due to the low porosity and permeability of oil and gas reservoirs (Hosseini 2016), the precipitation of $SrSO_4$, $BaSO_4$, and $CaSO_4$ is significant (He et al. 2014). These precipitates markedly reduce reservoir permeability, with mixed sulfate scales preferentially accumulating at porous media inlets, while individual $BaSO_4$ scales deposit uniformly throughout pore structures (Naseri et al. 2015; Alhseinat et al. 2021).

Consequently, the trace elements Li^+ , Sr^{2+} , and Ba^{2+} are all good indicators of gas production and can be used to assess the productivity of CBM wells based on the concentrations of trace elements in the produced water.

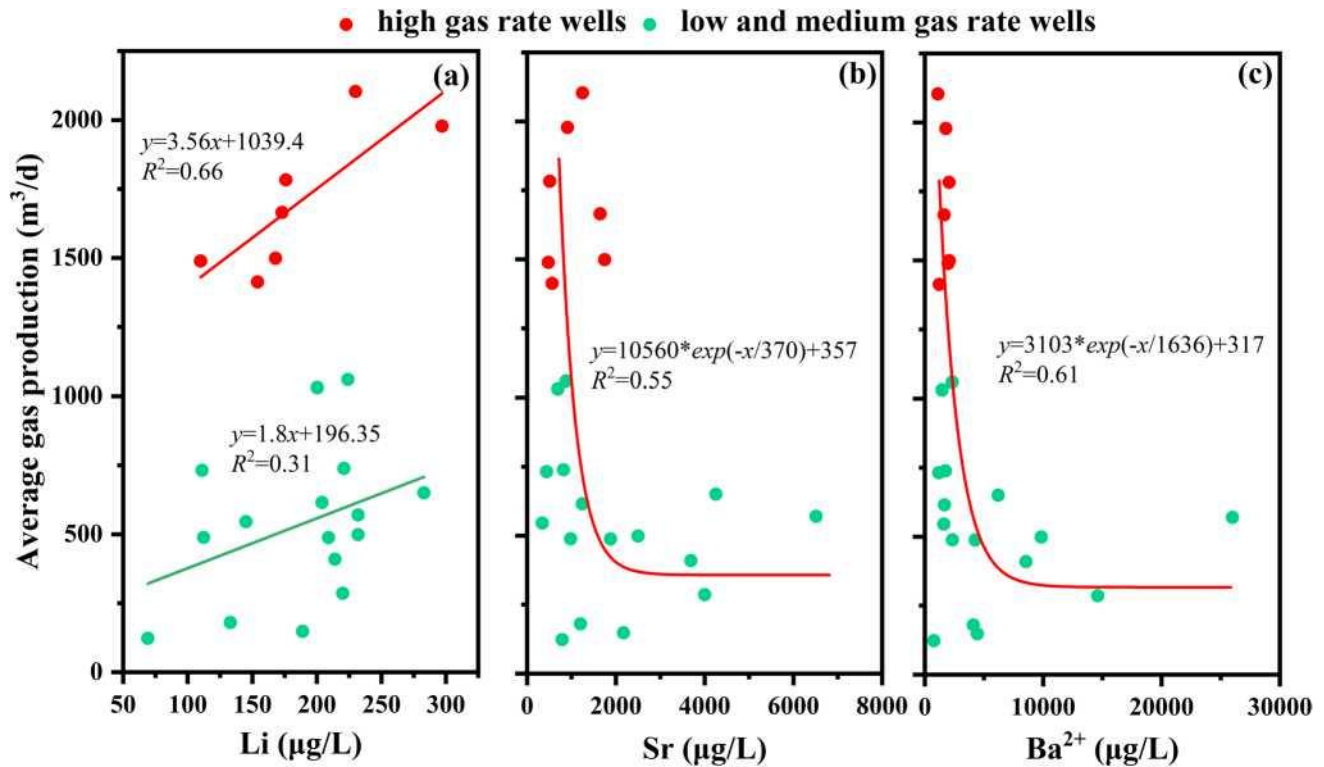


Fig. 15 Relationships between daily gas production rate and a Li^+ , b Sr^{2+} , and c Ba^{2+} with high and low gas rate wells

Isotope productivity response

Analysis of the relationship between hydrogen and oxygen isotope composition and gas production reveals that Z-5, C-1, X-11, and X-15, which all have high gas production, exhibit lower hydrogen and oxygen isotope composition, while X-17 and X-19, which have lower gas production, exhibit higher δD and $\delta^{18}O$ values (Fig. 16a).

Gas production tends to decrease with increasing hydrogen and oxygen isotope composition, showing a negative correlation between the two (Fig. 16b). Further analysis reveals that the low permeability of the Gujiao block coal seams (Feng 2018; Xia et al. 2019), combined with extensive fracturing fluid injection and low return rates, leads to the retention of fracturing fluid in the coal seam, resulting in strong water–rock interactions and continuous enrichment of hydrogen and oxygen isotopes. The high hydrogen and

oxygen isotope composition is attributed to the closure of the formation and the retention effect of the fracturing fluid, while the effect of evaporation leads to isotopic fractionation, resulting in the enrichment of heavy hydrogen and oxygen isotopes in surface water, and ultimately leading to lower gas production. Based on the analysis of the deuterium excess parameter d -value of groundwater in the previous section, a comparison with daily gas production reveals a significant relationship between the deuterium excess parameter d -value and the daily gas production of CBM wells. Gas production increases exponentially as the d -value increases. Wells Z-5, C-1, X-11, and X-15 have higher d -values, indicating higher gas production, while wells X-14 and X-19 have lower d -values and lower gas production (Fig. 16c).

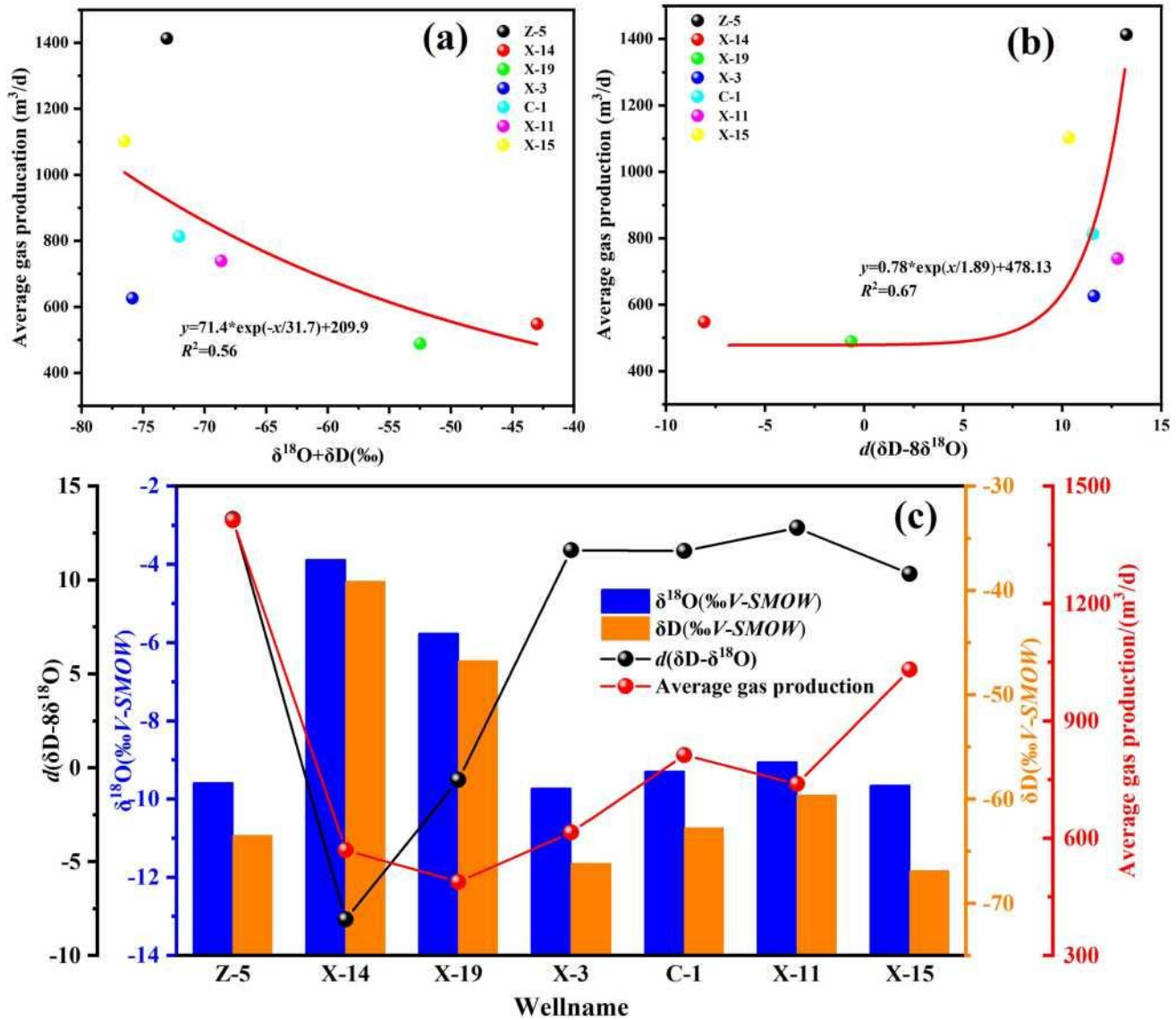


Fig. 16 The relationships between average gas production and a $\delta D + \delta^{18}O$, b $d(\delta D - \delta^{18}O)$, c δD , $\delta^{18}O$, $\delta D + \delta^{18}O$, d $(\delta D - \delta^{18}O)$ in different

The d -value often reflects groundwater flow conditions, as discussed in Section "Hydrogen and oxygen isotope characteristics". Based on the understanding of hydrogen and oxygen isotopes, the hydrogen and oxygen isotope composition and the deuterium excess parameter d -value of groundwater are closely related to gas production potential, and can serve as water chemistry indicators for evaluating gas production potential.

Productivity response mechanism of geochemical indices of produced water in CBM wells

The interaction between coal bed formation water and rock from the strong hydrodynamic area of exposed water supply to the final retention of the weak hydrodynamic area during the runoff process will have many effects on the gas production capacity of reservoirs. This section reveals the control mechanism of CBM well geochemical indicators in the Gujiao block from the perspective of well profiles, and presents a summary model for the processes in Fig. 17.

Atmospheric precipitation is delivered to coal seams through surface exposures, leading to lateral and vertical runoff in the formation, and allowing the water to interact with the coal beds and host rock matrix. Soluble evaporites and silicates dissolve, increasing the concentrations of Na^+ , K^+ , Ca^{2+} , Mg^{2+} , Cl^- , and SO_4^{2-} ions in the formation water.

There is a high O_2 content in the shallow part of the formation. Here, strong oxidizing conditions cause oxidation of minerals in the coal seam and surrounding rocks. The pH gradually decreases with depth, causing dissolution of carbonates and sulfates. The mineral CaCO_3 easily captures Sr^{2+} , leading to increased concentrations of Ca^{2+} , Mg^{2+} , Sr^{2+} , Ba^{2+} , and SO_4^{2-} in the water. Low-productivity areas often occur in high water level areas, where high concentrations of Ca^{2+} , Mg^{2+} , Sr^{2+} , Ba^{2+} , and SO_4^{2-} tend to form precipitates that block microfractures, impair reservoir permeability, and restrict gas production. However, the relationship between Ca^{2+} and Mg^{2+} and gas production is not significant. The study area has low-permeability reservoirs with high injection rates of fracturing fluid and low return rates, resulting in fracturing fluid retention in the coal seam. Strong water-rock interactions lead to continuous enrichment of hydrogen and oxygen isotopes, while evaporation causes isotopic fractionation, resulting in relatively higher concentrations of heavy D and ^{18}O in surface water, finally leading to lower gas production.

With the groundwater flow, due to the cation exchange adsorption, Ca^{2+} and Mg^{2+} , which have an adsorption capacity greater than Na^+ and K^+ , are more prone to water-rock interactions. High concentrations of Ca^{2+} and Mg^{2+} are extensively absorbed by the surrounding rocks, releasing the Na^+ and K^+ adsorbed by the rocks into the groundwater. When entering a weak hydrodynamic environ-

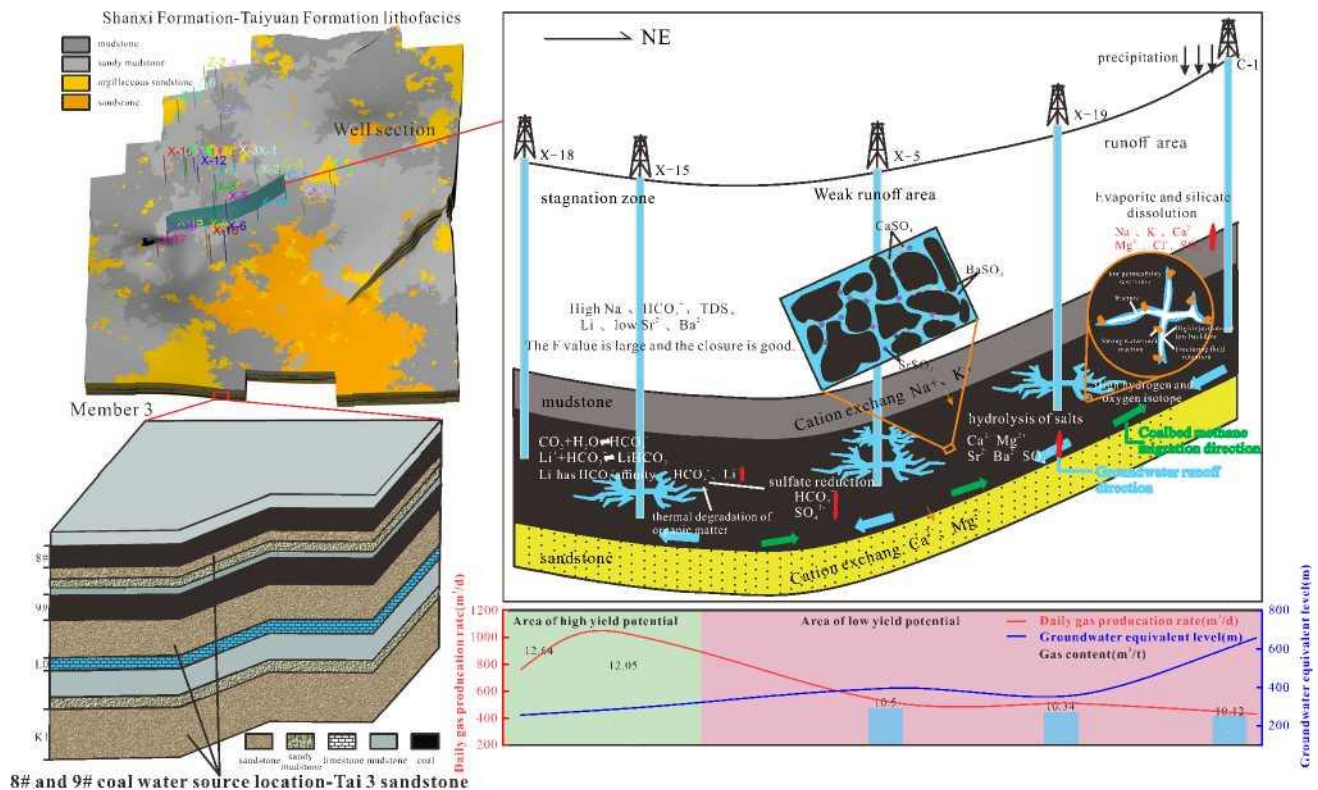


Fig. 17 Coal seam water geochemical index production control mechanism diagram

ment, microorganisms reduce SO_4^{2-} , leading to an increase in HCO_3^- content.

Moreover, the Gujiao block in has high concentrations of Na^+ and Cl^- in formation water, similar to formations in the Uinta and Alberta basins (Zhao et al. 2022). Thermogenic gas content is higher than biogenic gas content, and the dissolution of CO_2 during the thermal degradation of organic matter results in an increase in HCO_3^- concentration. The atomic radius of Li^+ is relatively small, showing a certain association with HCO_3^- , indicating a certain affinity for bicarbonates as Li^+ concentration increases. Additionally, an analysis of gas content in the study area reveals a good correlation between gas content and gas production, indicating that gas migration in coal seams is opposite to the direction of runoff, leading to trapping near areas of high gas potential, which is one of the reasons for higher gas production.

In the end, under the same well type, high gas production capacity wells often exhibit high levels of Na^+ , HCO_3^- , TDS, F^* , Li^+ , and d -value (deuterium excess parameter); while low levels of Sr^{2+} , Ba^{2+} , and $\delta\text{D} + \delta^{18}\text{O}$ (hydrogen and oxygen isotope composition) are typically observed.

This is an extremely complex set of inter-related geological, geochemical and geophysical phenomena and mechanisms, all of which combine to control production rates from CBM prospects.

Conclusions

- (1) The groundwater is predominantly of the Cl-Na type, originating from salt rock dissolution and cation exchange. δD - $\delta^{18}\text{O}$ signatures indicate sluggish groundwater flow conditions and confirm that sandstone aquifers are the main source of the produced water. The Sr^{2+} is derived from the dissolution of calcium-bearing minerals, with Ba^{2+} enrichment governed by the transitional marine-continental sedimentary facies of the Taiyuan Formation.
- (2) We established quantitative identification criteria for fracturing fluid contamination ($\text{Cl}^- < 70 \text{ meq/L}$ and $\text{K}^+ + \text{Ca}^{2+} + \text{Mg}^{2+} < 2.5 \text{ meq/L}$), excluding 29% of contaminated samples. Analysis of aquifer characteristics confirms that the produced water in CBM wells was sourced from the Member 3 Formation sandstone.
- (3) Gas productivity is governed by hydrogeochemical processes. In low-yield areas, strong hydrodynamics drive ionic precipitation that flow channels, while low permeability and trapped fracturing fluids enrich isotopes and limit production. Groundwater flow promotes

cation exchange (enriching Na^+ , K^+) and processes like sulfate and CO_2 dissolution, boosting HCO_3^- and Li^+ . High-yield wells are thus marked by high Na^+ , HCO_3^- , TDS, F^* , Li^+ , and d , as well as lower Sr^{2+} , Ba^{2+} , and $\delta\text{D} + \delta^{18}\text{O}$.

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