Chemical composition and formation conditions of NaHCO₃ type of waters in the eastern Transbaikalia

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Abstract. The chemical composition of the supergene zone groundwater in the Eastern Transbaikalia is considered. The main geochemical processes for steppe landscapes are identified and determined the causes of some component's concentrations in groundwater. To understand the formation conditions of NaHCO₃ water, were calculated equilibria of this water with the main minerals of the region’s rocks.

1 Introduction

NaHCO₃ type of waters due to the uniqueness of their composition have given rise to particular debates among scholars. Therefore, the elucidation of their formation is one of the fundamental problems in hydrogeochemistry. This problem has discussed for a long time in the works of domestic [1-6] and foreign [7-8] researchers but many of its aspects are far from being clarified.

The main task of our study was to highlight the main points of NaHCO₃ water formation in the region based on chemical composition data and thermodynamic calculations.

2 Materials and methods

2.1 Study Area

The studied waters are localized within the Torean artesian basin [9] belonged to the Mongolian type and characterized by low mountain framing, Lower Cretaceous and Cenozoic sedimentary cover and the absence of runoff.

Depending on the nature of groundwaters in the host rocks and taking into account their age among the studied water manifestations two aquifers could be distinguished: a reservoir type and fissure waters.

Water bearing stratum of loose Quaternary deposits with a reservoir type of accumulation is common in alluvium floodplains and terraces. The water-bearing soils are

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sand, gravel, sandy loam. Cretaceous host rocks of fissure waters are represented by terrigenous and terrigenous-volcanogenic sediments consisting of pebbles, boulders, conglomerates, gravelites, sandstones, siltstones, tuffaceous varieties, effusives and lignite beds.

The piezometric level of the studied water seepage was at a depth from 4 to 80 m, and sometimes was above the earth surface. The water temperature varied from 2 to 7 ºC.

![Fig. 1. Sketch map of the studied area showing the sampling points.](image)

**2.2 Sampling and Analysis**

The water samples for major components stored in 1,5 L clean polyethylene bottles, and the samples for minor components analysis were stored in 50-mL bottles. All tanks were pre-washed with the samples water. Measurements of the Eh and pH of natural solutions were performed by anionomers CG 837 (Schott), Anion 7000 (Infraspack-Analyte) and combined electrodes Platin Elektrod Blu Line 31 RX and ESK 10061 on-site.

Laboratory studies included determination of the (CO$_3^{2-}$, HCO$_3^-$, SO$_4^{2-}$, Cl$^-$, F$^-$, Ca$^{2+}$, Mg$^{2+}$, Na$^+$, K$^+$) by potentiometric methods, atomic emission, flame absorption, and Si by colorimetric methods.

The chemical test was carried out in the certified laboratory of geocology and hydrogeochemistry of the Institute of Natural Resources, Ecology, and Cryology (Siberian Branch, Russian Academy of Sciences) and Fundamental Research Laboratory of Hydrogeochemistry of Research and Education Centre “Water”.

The physicochemical modelling program HydroGeo [10] was used to calculate the ion activities in the natural waters. The diagrams of some secondary and primary mineral stability fields were used to show the water saturation state with respect to basic mineral phases.

**3 General characteristics of waters**

The diversity of the chemical composition and the Total Dissolved Solids are a distinctive feature of the groundwater of the territory under consideration (Table).

As the absolute elevation decrease, the increase in TDS is more often observed. Therefore, groundwater with the TDS more than 1,0 g/L is distributed in the southern part of the territory, on the catchment area of the largest soda lakes Barun- and Zun-Torey, and more fresh waters are concentrated in the north-west and northeast of the region (Fig. 1).
In general, as the TDS and pH increase, Na$^+$, HCO$_3^-$, CO$_3^{2-}$, Cl$^-$ and SO$_4^{2-}$ accumulate. On the contrary, the contents of Ca$^{2+}$ and Mg$^{2+}$ decrease. The following sequence of conversion of groundwater is revealed as their TDS increases they transfer from hydrocarbonate with mixed cationic composition to sodium hydrocarbonate, i.e. soda.

### 4 Water-rock interaction

First of all, consider the equilibrium of water with carbonate minerals. As can be seen in the diagrams, the rock dissolution occurs under conditions of the saturation of groundwater with calcite. At the same time, precipitation remain non-equilibrium with calcite (Fig. 2). It turns out that for the formation of calcite it is necessary to follow conditions, i.e. the TDS of water was not lower than 0,4 g/L, pH> 7,7, and the content of HCO$_3^-$ was more than 0,1 g/L.
Fig. 2. Calcite (1), dolomite (2) equilibrium diagram (e) at 25°C and 1 bar.

With increasing TDS (> 0.6 g/L), pH (> 8.2), carbonate content (> 0.3 g/L), and amounts of Ca²⁺ and Mg²⁺ (> 0.02 g/L), groundwater comes to an equilibrium with dolomite and magnesite. At the same time, all natural waters remain unbalanced with gypsum, fluorite, gaylusite, and halite.

In addition to the considered secondary carbonate and sulphate minerals, the equilibrium of water with aluminosilicate and silicate minerals was studied. For these purposes, the classical $\log [H_2SiO_4] - \log [Me^{+} / H^{+}]$ diagrams were used, where Me is K⁺, Na⁺, Ca²⁺ and Mg²⁺ [8].

Thus, precipitation occurs at the stage of gibbsite formation. Most of the points related to groundwater are located in the stability fields of montmorillonite and illite. With increasing of TDS (> 1.0 g/L) and pH (> 8.3), water comes to equilibrium with Mg-chlorite, and with TDS more than 2.0 g/L and pH > 8.5 with prehnite and albite.

Fig. 3. Selected activity diagrams in $H_2O$-$Al_2O_3$-$Na_2O$-$CO_2$-$SiO_2$ (1); $H_2O$-$Al_2O_3$-$MgO$-$CO_2$-$SiO_2$ (2); $H_2O$-$Al_2O_3$-$K_2O$-$CO_2$-$SiO_2$ (3); $H_2O$-$Al_2O_3$-$CaO$-$CO_2$-$SiO_2$ (4) systems at 25°C.
The presence of loose Quaternary deposits (sands, sandy loams, pebbles, etc.) in the studied area provided the conditions under which precipitation quickly penetrates into deeper lithified Mesozoic rocks. A part of the water penetrates into the basement rocks, thereby ensuring the duration of interaction with aluminosilicate rocks. As groundwater moves to the discharge areas, NaHCO\textsubscript{3} type of water actively begins to form in troughs, where, in combination with intensive capillary evaporation and stagnant regime, additional conditions of water salinization are created.

As the result (as equilibrium is achieved), calcite, magnesite, dolomite and clay (kaolinite, montmorillonite, etc.) are formed that reduces the contents of Ca, Mg, K and other elements in the solution. In contrast, Na will accumulate throughout the process, as it is associated with mineral formations in small quantities, compared with its quantity in the bed rock.

5 Conclusion

The sample analysis showed that an increase in the content of Na is accompanied not only by an increase in salinity, but also an increase pH, which is mainly due to the hydrolysis reactions of aluminosilicates and, as a result, the appearance of OH\textsuperscript{-} in waters [1], which participates in the HCO\textsubscript{3}\textsuperscript{-} formation reaction. At the same time, Cl\textsuperscript{-} and SO\textsubscript{4}\textsuperscript{2-} are concentrated in waters, as there are no geochemical barriers that limit their content in waters.

The closed nature of the Torey depression, the absence of surface and groundwater runoff, a significant lack of moisture, intensive evaporation all collectively determine the stagnant water regime and relatively high TDS, the pH value and the content of many chemical elements.

The work was supported by Russian Foundation for Basic Research Project № 18-05-00104 A and Russian Science Foundation Project № 17-17-01158.

References
1. S. Shvartsev, Geochemistry of fresh groundwater in the main landscape zones of the Earth. Geochem Int 46(3), 1285-1398 (2008)
2. Y. Posokhov, The origin of soda water in nature (1969) (in Russian)
3. V. Sulin, Hydrogeology of oil fields (1948) (in Russian)
4. S. Durov, Synthesis in hydrochemistry. The origin of the salt composition of natural waters (1961) (in Russian)
5. M. Valyashko, Geochemistry and genesis of brines of the Irkutsk amphitheater (1965)
6. S. Krainov, B. Ryzhenko, V. Shvets, Groundwater geochemistry. Theoretical, applied and environmental aspects (2004) (in Russian)
7. J. Drever, The Geochemistry of Natural Waters: Surface and Groundwater Environments (3rd Edition) (1997)
8. H. Helgeson, Evaluation of irreversible reactions in geochemical processes involving minerals and aqueous solutions – I. Thermodynamic relations, Geochim. Cosmochim. Acta, 32, 853-877 (1968)
9. A. Verkhoturov, V. Tsyganok., V. Karpov, L. Vasyutich, E. Belyakova, Hydrogeology of the Transbaikal Region (2017) (In Russian)
10. M. Bukaty, Software development for solution of hydro-geological problems 305, 348-365 (2002) (In Russian)