Singenetic waters composition reconstruction methods of mesozoic sedimentary basins

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Abstract. In the article the methods of singenetic waters composition reconstruction of Mesozoic and Cainozoic sedimentary basins based on naturalhistorical approach is presented. The average concentration of the main macrocomponents of waters buried both sea, and continental conditions are given. Example of application of the methods in Arctic basin is done.

1. Introduction

The analysis of macro- and microcomponent composition of groundwater makes it possible to reveal the hydrogeochemical zonality, to determine the paths of vertical migration of fluids, and to tentatively determine their genesis. However, present-day groundwater chemistry radically differs from that of syngenetic waters, buried simultaneously with sediments at the elision and infiltration stages of basin development. To understand the nature of groundwaters chemical composition and hydrogeochemical zonality requires paleohydrogeochemical reconstructions, making it possible to assess the effect of diagenetic and catagenetic changes and the processes of interaction in the water–rock–gas–organic matter system on transformations in groundwater chemistry during the evolution of the sedimentary basin.

2. Materials and methods

The procedure for the reconstruction of water salt composition in ancient marine and lake–alluvial basins is based on paleogeographic reconstructions and comparative–lithological analysis with naturalhistorical approach, the essence of which is the assumption that the formation of ion–salt composition of water in continental and marine environments in the past geological epochs was governed by the same factors and determined by the same processes as in the present time. Two groups of factors determine the direction of changes in water chemistry in the course of geological evolution of a sedimentary basin: (1) the factors that determine the genetic type and composition of original water, i.e., the lithological–facial, paleographic, and paleoclimatic, and (2) the factors that govern the changes in groundwater chemistry after its burial, i.e.,the temperature, pressure, dynamics, and geochemistry of the environment, as well as the effect of infiltration recharge. To analyze the development of a confined groundwater system throughout the period of its existence requires a periodization of the hydrogeological history [14]. It is based on the assumption that, in any region, one or several hydrogeological cycles can be identified, consisting of elision and infiltration stages. At the initial (elision) stage, transgression of the sea basin is taking place. In this time, sedimentogenic water is buried along with thalassogenous sediments and the processes of elision water exchange are predominant. At the final (infiltration) stage, which corresponds to regression, meteogenic (infiltrogenic) water enters the lithosphere and partially replaces and displaces the sedimentogenic water that has accumulated before. Starting from the stage of the burial of syngenetic water, the process of transformation of its chemistry begins, governed, first, by sedimentation environments and next, at the stages of diagenesis and katagenesis, the processes of vertical and lateral migration and interaction in the water–rock-gas–OM system. This means that the initial composition of sedimentation waters can be derived from the sediment formation conditions. The increase in the total salts in continental environments is taking place mostly due to hydrocarbonate ion and calcium; while that in marine environments, due to ions of chlorine, sodium, and magnesium. Magnesium is an indication to the deepwater environments of silt-water accumulation.

To reconstruct the composition of waters of ancient marine basins (elision stages), data on the modern chemistry of the ocean [1, 18], silt water [22], and absorbed clay complex [8, 9, 21] were generalized. The initial composition of infiltration water (continental sedimentation environments) was reconstructed by the average composition of river, bog, and lake water and the geochemistry of the hypergenesis zone [7, 23]. In addition, the results of paleontological and paleoclimatic studies were used to determine the mean annual temperature and salinity in the Boreal Basin [3–6, 10–13, 17, 19, 20, 24]. Paleoclimatic reconstructions are based, primarily, on studying the spore–pollen complexes, the occurrence of benthic forms, isotopic thermometry (δ18O and δ13C), and the Ca/Mg ratio in the shells of marine organisms. The present-day studies show that the Mesozoic era was a period of greenhouse climate, though, with some zonality. The zone under consideration lied in the moderately warm boreal climate zone with a passage into subtropic zone. The seas of high paleolatitudes, in addition to boreal species, were periodically inhabited by subtropic and tropic mollusks; and the land, by tropic plants [10]. Against the background of relatively high mean annual temperatures, typical of the Mesozoic, short-time but, sometimes, wide temperature variations were taking place (5–6°C). The temperature of surface layers and shallow water varied from +11 to +24°C, while the bottom waters of the deep parts of the shelf were cooler [24].

Paleontological data confirm that the salinity in the epicontinental shallow seas of the Arctic was close to that of the ocean (35 g/dm^3); however, water in coastal zones was freshened (<18 g/dm^3) by continental runoff, especially, in the periods of climate humidization.

Studies of the composition of the modern sea (the seas of Okhotsk, Japan, Baltic, White, and Caspian) and oceanic waters suggest that the maximal salinity of the buried waters of Mesozoic basin could not be higher than 38 g/dm^3 in the deepest marine environ ments, while in shallow and coastal zones, it could vary from 10 (freshwater inflow from rivers) to 25 g/dm^3.

In terms of composition, chloride sodium water dominated, with an increase in magnesium with deepening of the sea basin.

Detailed analysis of the results of studying continental and coastal-marine sediments in the environments of semiarid climate has shown that infiltration water exchange caused the formation of fresh, mostly hydrocarbonate calcium waters with a total mineralization of up to 0.5 g/dm^3 and the formation of brackish waters (up to 10 g/dm^3) in the coastal-continental environments. The characteristics of the mean composition of syngenetic waters of different facial zones of the West Siberian paleobasin are giver in Table 1.

3. Results and discussion

The methods has been successfully approved in the Arctic region (Gydan, Pur-Taz, Yenisei-Khatanga, Anabaro-Hatanga, Lena-Anabar and Laptev see oil-and-gas- bearing regions and in the southern region of the West Siberian basin (Kaymysovsky and Vasyugan regions).

Let's consider history of formation of sedimentary deposits during Jurassic and Cretaceous period of eastern part of Bol’shekhetskaya Megasyneclise (west part of Yenisei-Khatanga megatrough) by way of example.

The vast transgression, which started at the Carnian stage of Triassic, caused the formation of a shallow marine basin in the northern West Siberia. The examined region contained a vast transition zone—a coastal plain, inundated by the sea from time to time [2, 16].

Table 1. Average composition of syngenetic waters of marine and continental sedimentation environments in northern regions of the West Siberian basin in the Mesozoic and Cenozoic.

Facial environments	M_{av}*	Elements						
		SO_4^{2-}	Cl^-	HCO_3^-	Na^+	K^+	Ca^{2+}	Mg^{2+}
Continental	mg/dm^3							
Mountains, elevated plain	65.0	2.4	5.7	35.0	11.0	1.4	3.2	1.7
Floodplain–bog	44.0	3.0	3.5	25.0	3.0	0.8	6.5	1.5
Lacustrine–alluvial	150.0	10.0	7.0	55.0	5.1	1.3	14.0	4.0
Marine	g/dm^3							
Coastal-marine	17.5	1.2	8.2	0.3	6.2	0.1	0.4	1.1
Deep-sea–marine	34.5	2.7	18.9	0.14	10.5	0.3	0.4	1.3

*M_{av} is mean mineralization.

This zone with moving shoreline showed the formation of coastal-marine and continental sediments with remains of deciduous flora and plant detritus. In addition, because of the unstable marine regime, water salinity in the paleobasin varied from 2 to 20 g/dm^3.

The composition of sedimentary formations that formed in the Late Triassic in Siberia territory suggests that, in that period, the study area lied within the moderate belt (boreal) with relatively warm and wet climate and mean annual water temperature reaching +20°C, which persisted until the Early Jurassic [21].

Since the early Jurassic (Hettangian), the marginal Siberian basins were at the transgression stage of their development caused by level rise in the seas of the Boreal Basin [12]. The deepest northwestern part of the examined region was inundated by a shallow (up to 25 m) sea. In this area, marine sediments have deposited with predominantly chloride sodium water with a high concentration of hydrocarbonate ion and calcium and with mineralization of 10–20 g/dm^3. In the eastern direction, the basin became shallower, and the sedimentation environments changed from coastalmarine to continental, where the processes of fresh atmospheric water infiltration predominated (Fig. 1a).

Such environments persisted up to the beginning of Toarcian, when, after an insignificant Late Pliensbachian regression, a transgression of sea basin, largest in the Middle Jurassic, took place. In this period, fine washed clays of kiterbyut formation formed [26]. The major portion of the examined region was a shallowsea basin with depths to 100 m; water salinity could reach 25 g/dm^3. The Early Toarcian showed warm climate with mean annual temperature estimated by oxygen isotope composition in belemnite rostra at +16.9– +24.5°C; this temperature caused a bloom of various marine fauna, especially, belemnites and ammonites, in the Arctic seas [19].

The second part of the Early Toarcian and the beginning of Aalenian featured a general short but vast regression of Siberian seas, resulting in a shallowing and freshening of the marine basin. Nevertheless, the contours of the main paleogeographic zones kept unchanged up to Callovian. The gradual cooling (down to +15°C) and moistening of the climate in the second part of the Aalenian caused the death of vegetation and, consequently, a wide occurrence of carbonaceous strata and the appearance of arctic genera of ammonites and belemnites in the basin [3, 12, 19].

In the Bajocian, short-time rises (in the beginning) and lowering (in the end of the century) of the sea level took place, which have no considerable effect on the position of paleogeographic zones [16]. The climate in the Bajocian was also cool and humid, the mean annual temperatures were +14–+16°C [3].

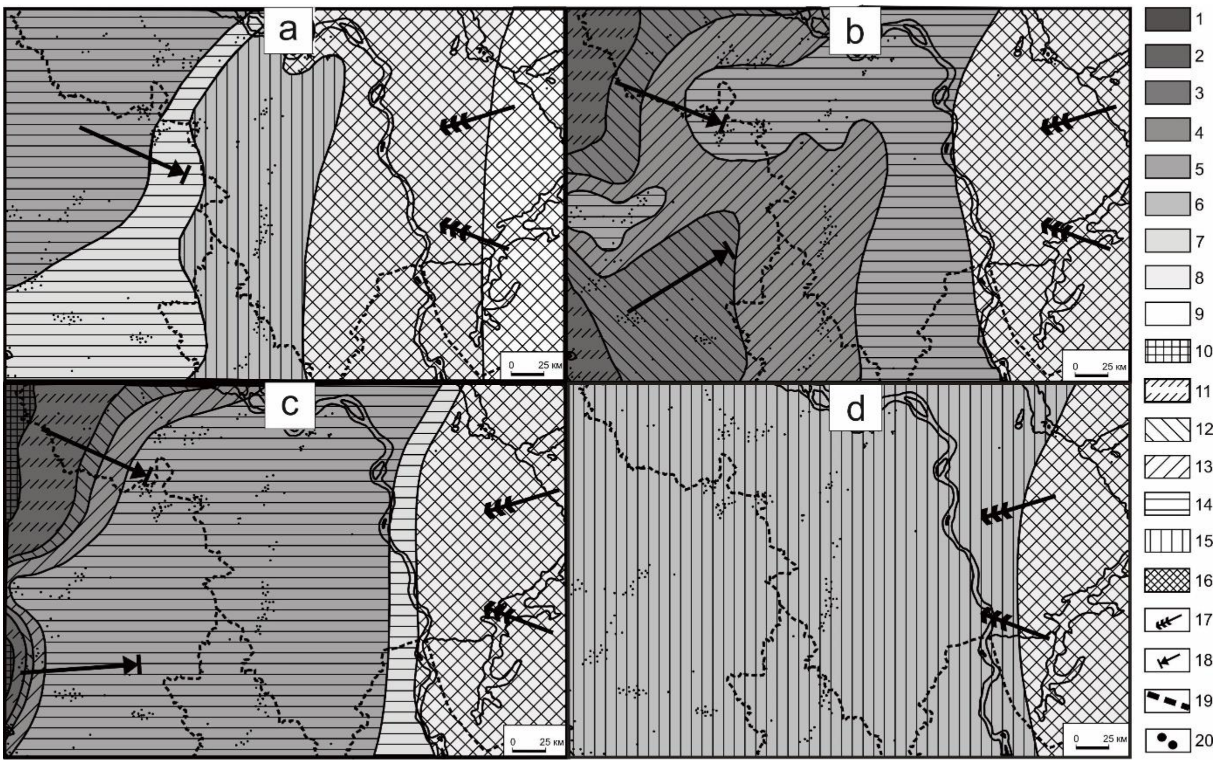

Figure 1. Paleohydrogeochemical scheme with elements of facial zonality and the modern hydrogeochemistry of the northeastern part of Bol'shekhetskaya Megasyneclise at the beginning of (a) Pliensbachian, (b) Volgian, (c) Valangimian, and (d) Aptian ages (paleogeographic data are based on materials of [2, 12, 15, 16]).

Sedimentation environments: (*1*) deep sea, continental slope (>400 m); (*2*) sea, deep part of the shelf (200–400 m); (*3*) sea, outer part of the shelf (100–200); (*4*) sea, internal part of shelf (25–100); (*5*) coastal zone, insular and beach parts of the shelf (0–25 m); (*6*) lowland accumulative plain; (*7*) coastal plain, inundated by the sea from time to time; (*8*) denudation elevated plain; (*9*) low maintains, plateau; paleohydrogeochemical burial zones of (*10*) salt (talassogenic) waters with mineralization of 35.0–38.0 g/dm^3 with the predominance in the composition of Cl^- and Na^+ at higher Mg^{2+} concentration (deep-water marine environments); (*11*) salt (talassogenic) water with mineralization of 25.0–35.0 g/dm^3 with the predominance in the composition of Cl^- and Na^+ ions at higher Mg^{2+} concentrations (marine environments); (*12*) salt (talassogenic) water with mineralization of 20.0–25.0 g/dm^3 with the predominance in the composition of Cl^- and Na^+(shallow-water marine environments); (*13*) salt water with mineralization of 10.0–20.0 g/dm^3 with the predominance in the composition of Na^+ and Cl^- at higher concentration of Ca^{2+} ions (coastal-marine environments); (*14*) salt waters with mineralization of 2.0–10.0 g/dm^3 with the predominance in the composition of Cl^- and Na^+ at higher concentration of and Ca^{2+} (coastal-continental environments); (*15*) fresh and brackish infiltrogenic water with a mineralization of 0.5–2.0 g/dm^3 and with the predominance in the composition of and Ca^{2+} ions at higher concentration of Cl^- and Na^+ ions (continental environments); (*16*) fresh infiltrogenic water (with the predominance of meteogenic) with mineralization from 0.5 g/dm^3 with the predominance in the composition of and Ca^{2+} ions (continental environments); the main directions

of motion of (*17*) infiltration water and (*18*) elision water; other: (*19*) administrative boundaries; (*20*) wells.

In the Bathonian age, the positions of the zone of marine sedimentation did not change, but the periods of sea ingressions increased. In addition, the paleontological data suggest a new wave of warming, which led to the formation of subtropic humid climate on the northern West-Siberian

Lowland. This can be seen from the development of glauconitic sediments and coccolithophorids among algae [19].

The Callovian stage shows the beginning of a vast sea transgression, resulting in the deepening of the sea basin down to 200 m in the west of the region, where fine clay sediments with abundant fauna were accumulating. In this part of the sea basin, water salinity reached 30 g/dm^3. The fauna that inhabits the arctic basin becomes more diverse because of the continuing warming (water temperature increased by 2–3°C), and thermophilic species appear. At the passage from the Callovian to Oxfordian ages, the transgression gave place to regression, which continued until the mid-Oxfordian stage. The deeper zone shifted into the extreme northeastern part of the region, and the shallow zone (25–100 m) extended considerably with clay and sand–aleurite–clay sediments accumulating within it. The morphology and boundaries of the coastal–marine zone (with the sea depth of < 25 m) has changed insignificantly since the

Callovian age. The coastal plain, located in the southern part, was inundated by the sea [2, 16].

The transgression continued over the Volgian age and reached its maximum in the middle of the century (Fig. 1b). The climate in the Volgian age was nearly semiarid, resulting in the predominance of chemical weathering processes on the continent and the accumulation of mostly clay and organogenic rocks on the shelf [9, 12, 16, 21]. By the end of the Volgian age, a deep paleobasin of underbalance type with signs of hydrogen-sulfide pollution has formed in West Siberia. The study area was inundated by a sea of Late Jurassic transgression with depths of 400 m in the extreme northwestern and southwestern parts, where water salinity reached 35–38 g/dm^3. A zone with depths of 100–200 m formed near the Khal'merpayutinskaya area, where salt thalassic waters with mineralization of 20–25 g/dm^3 and the predominance in the composition of chlorine and sodium ions and higher magnesium concentration were buried along with marine sediments. The major area of the Khatanga marine basin with depths from 25 to 100 m has decreased from the Bathonian to the Oxfordian and, in the Volgian time, it lied as narrow belts along the contour of the deeper domain. The contours of the coastal zones have not changed. In the end of the Volga and the beginning of the Berriasian, a temperature drop by 4–5°C took place, maybe locally, in Northern Siberia. In the Late Berriasian, Valanginian, and early Hauterivian, the seas were still warm, somewhat cooler than they were in the Kimmeridge–Volgian time. This is confirmed by the diversity of the fauna (large bivalves and oysters and the spore–pollen complex (tropical ferns), suggesting subtropic humid climate [19]. Paleobiogeochemical analysis of oyster shells shows that water paleosalinity of the Khatanga Sea in the Early Berriasian age was close to that of the ocean (35 g/dm^3), reaching 32 in the Valanginian period and 31 g/dm^3 in the Hauterivian [18].

In the early Berriasian age, a depression with depths not greater than 400 m formed in the southwestern part of the region because of an increase in the rate of basin warping and not enough precipitation for its compensation [15]. The contours of other zones remained almost unchanged. In this time, the sea basin was connected with boreal seas and its water salinity in the deepest parts was close to that of the ocean.

In the Early Valanginian, the regression that began in the late Jurassic still kept developing (Fig. 1c). This has led to the formation of a vast shallow zone with depths <25 m. In the coastal zone, along with beach sediments, brackish water with mineralization of 10–20 g/dm^3, with the predominance in its composition of ions of chlorine and sodium and with higher calcium concentration because of the inflow of fresh meteogenic waters from the continent, was buried. A deep-water depression with a small area persisted in the northwestern part of the region. A coastal plain, inundated by the sea from time to time, formed again in the eastern part. The climate in the Hauterivian was humid and moderate, with mean annual water temperatures reaching +17°C. The West-Siberian Basin lost its connection with the boreal seas because of its further shallowing; its water also became much fresher [15]. In the examined area, the shallow zone became a vast coastal plain where floodplain, delta, and beach environments alternated, depending on the sea level, and brackish water with mineralization of 2–10 g/dm^3, chloride sodium composition, and higher concentration of hydrocarbonate ion and calcium was buried. Warm subtropical climate also existed in the West Siberian Plain in the second half of the Early Cretaceous, though with much higher humidity, facilitating the deeper decay of sedimentary material [19]. Under such conditions, bauxite deposits and thick coal-bearing strata were forming. Starting from Barreme and up to the Late Cenomanian, environments of a lowland accumulative plain and a coastal plain were alternating [15]. Under such conditions, infiltration meteogenic hydrocarbonate-calcium water with mineralization of up to 2 g/dm^3 was mixing in the zone of active water exchange with sedimentogenic waters, partially diluting and freshening them (Fig. 1d).

The further transgression, which started in the Turonian age, caused the formation of a vast shallow zone, covering the entire examined area up to the Late Campanian. Seawater salinity could reach 20 g/m^3 in deepest parts in the southwestern part of the region. In the Late Cretaceous epoch, the climate conditions generally somewhat deteriorated, as can be seen from the composition of marine fauna inhabiting the Arctic Basin, a single species of bivalve dominated, and rare belemnites and ammonites could be met [19]. The further temperature drop contributed to the formation of siliceous rocks (gaizes) in the Coniacian– Campanian. The Late Campanian showed a regression of the sea basin and warming of the West Siberian Sea, resulting in the deposition of calcareous sediments and an increase in the coastal plain area. In this period, dominating in the syngenetic waters in the coastal–continental environments were infiltrogenic hydrocarbonate calcium waters with higher concentration ofsodium and chlorine ions and mineralization reaching 10 g/dm^3.

4. Conclusion

The present-day formation water is a product of the geological evolution of the sedimentary basin. The sedimentogenous and ancient infiltrogenic water serve as a source of two major geochemical branches of waters widespread in the Arctic region. Further, their composition experiences radical changes; once in the sedimentary basin, they become involved in many processes of interaction in the water–rock–gas–organic matter system, experience diagenetic and katagenetic transformations, and mix with one another in different proportions. The genetic coefficients and paleohydrogeochemical reconstructions can be used to determine the nature of groundwater and to assess the changes that have taken place in its chemistry in the geologic time.

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