Paleohydrochemistry of Jurassic and Cretaceous deposits in arctic regions of Western Siberia

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Abstract. The Jurassic and Cretaceous paleohydrogeology of the Arctic regions of Western Siberia includes three hydrogeological cycles: Induan-Sinemurian, Pliensbachian-Cenomanian, Turonian-Serravallian. The paper presents results of the paleohydrological reconstructions of Jurassic and Cretaceous deposits. In the Triassic-Early Jurassic and Berriasien-Cenomanian, the continental regime of sedimentation was prevalent within the study area, along with the processes of infiltration of fresh meteoric waters mainly hydrocarbonate calcium in composition with the TDS value not exceeding 5 g/dm³. Marine sedimentation conditions were dominant during the Pliensbachian-Hauterivian and Turonian-Barronian elision stages, when the processes of sedimentation were accompanied by syngenetic burial of sodium chloride waters, locally rich in magnesium, with the TDS value reaching 35 g/dm³ in the deepest parts of the marine basin existing in the Volgian time. Modern chemistry of groundwaters of Jurassic and Cretaceous deposits in the Arctic regions of Western Siberia is a product of long-term geological evolution of the "water-rock-gas-OM" system.

1. Introduction

As a separate science, paleohydrogeology emerged early in the 20th century and studies the past stages in the development of sedimentary basins, aiming to clarify the role played by ancient groundwaters in the formation and preservation of mineral deposits, which was extensively discussed in the pioneer works of P.N. Chirvinskii. Later, this research line was largely contributed by many prominent scientists, among them L.A. Abukova, E.A. Baskov, E.A. Bars, S.B. Vagin, A.A. Kartsev, K.I., Makov, A.M. Nikanorov, E.V. Pinniker, A.N. Semikhato, Ya. A. Semikhato, Ya.A. Khodzhakuliev, S.A. Shagoyants, G.P. Yakobson and others. [1-3]. Given that paleohydrogeological studies are scant both in Russia and abroad, only few works devoted to sedimentary basins of Siberia, Eastern Pre-Caucasian, and the Pre-Kama Perm regions have been published recently [4-6].

Modern advanced-level scientific research requires aggregation of the latest data from many areas of the Earth Sciences, such as hydrogeology, lithology, stratigraphy, tectonics, etc. whose results and findings are helpful in solving many problems of modern hydrogeochemistry of oil and gas accumulations, including the composition of groundwaters, their origin, type of vertical hydrogeochemical zonality, the processes of petroleum generation and accumulation, and other aspects.
2. Materials and Methods

Paleohydrogeological studies of petroleum basins focus primarily on periodization of their hydrogeological history, consisting in determination of hydrogeological cycles and stages. According to A. A. Kartsev, S. B. Vagin and E. A. Baskov, a hydrogeological cycle begins with transgression and includes depositional processes with concomitant burial of sedimentary waters, spanning the period of subsequent elevation and regression, and culminates in a new submergence and transgression. The first part of hydrogeological cycle (from the start of transgression through the beginning of regression) is a sedimentary (elision) stage during which the formation of sedimentary waters and the elision water exchange take place. Its second part accounts for infiltration stage characterized by impoundment of waters of infiltration over the sedimentary basin progressively expulsing and replacing sedimentary waters [1].

Discrimination of elision cycles was largely based on the study of paleogeographic maps and lithofacies schemes, which provided the data on the predominantly marine regime of sedimentation. Infiltration cycles were determined from the data on the continental sedimentation regime existing in most of the study area, on the presence of hiatuses in sedimentation, inconformities, scours and basal layers of the overlying deposits [7-8]. Due to the inconsistencies between the boundaries of some cycles and those of large stratigraphic units (erathems, systems, divisions), their names were derived from their assignment to the generally accepted stages of the stratigraphic scale.

The restoration technique for the salt composition of waters from the ancient Mesozoic marine and lacustrine-alluvial basins is based on paleogeographic reconstructions and comparative-lithological analysis using natural-historical approach, which, in itself, is reduced to the fact that the formation of the ion-salt composition of waters in the continental and marine environments had common controls and are the product of identical processes occurring both in the past geological epochs and at the present time [9]. The paleohydrological reconstructions were based on the method for restoration of salt composition of waters of ancient Mesozoic marine and lacustrine-alluvial basins; by studies of paleogeographic maps of the Jurassic and Cretaceous periods compiled by the IPGG SB RAS researchers [6, 9], hydrogeological databank available at the IPGG SB RAS Laboratory for Hydrogeology of sedimentary basins of Siberia for the Arctic regions of Western Siberia, resulted from testing more than 3000 objects of 211 target areas, including the results of full chemical analysis of 3205 groundwater samples.

3. Hydrogeochemical signatures

Groundwaters with the TDS value varying from 2 to 63.3 g/dm³ and having different chemical composition were revealed within Jurassic and Cretaceous deposits of the Arctic regions of Western Siberia. The prevailing are Na Cl, Na Cl-HCO₃ and Na HCO₃-Cl water types (after Shchukarev S. A.), with each having its own patterns of main salt - forming macro-and micro components distribution, whose concentrations are dictated by their salinity levels: its growth directly entails an increase in Cl, Na, Mg, Ca, K amounts, as well as in micro components (Br, I, B, NH₄ and Sr). The amounts of hydrogen carbonate (bicarbonate) ions tend to decrease starting from water salinity 15-20 g/dm³ and more. The sulfate-ion concentrations do not exceed on average 20 – 60 mg/dm³, which is associated with the remarkable process of its reduction to hydrogen sulfide: $\text{SO}_4^{2-} + 2\text{C}_{org} + 2\text{H}_2\text{O} \rightarrow 2\text{HCO}_3^- + \text{H}_2\text{S}$.

The aquifer complexes (Aptian-Albian-Cenomanian, Neocomian, Upper Jurassic and Lower-Middle Jurassic) are marked by a number of hydrogeochemical signatures derived from the paleohydrogeological data [6], by subsequent processes of the groundwater chemistry metamorphization, as well as by the vertical migration of brines from Paleozoic basement to the overlying sedimentary cover in the areas of missing thick Triassic volcanic-sedimentary strata, acting as a desalinated "hydrogeochemical cushion" [10]. The anomalies in the hydrogeochemical field revealed in a number of areas in central areas of the study area accompany the process of inter-strata crossflows from the underlying sediments [11]. The diversity of groundwater composition observed at the base of the sedimentary cover generally decreases up the section, exhibiting significant smoothing of hydrogeochemical conditions and leveling of the groundwater salinity in the range from 15 to 20
g/dm³ in the Aptian-Albian-Cenomanian complex [10-13]. This can be exemplified by the considered below features of hydrogeochemistry of the upper Jurassic aquifer complex whose water salinity was found to be the highest.

Groundwaters of Upper Jurassic sediments are characterized by varied chemical composition with dominance of NaCl, NaCl-HCO₃ and NaHCO₃-Cl water types whose TDS values vary in a wide range—from 5 to 63.3 g/dm³ [10-16]. With increasing salinity, the chemical type of water changes from sodium bicarbonate chloride to sodium chloride (figure 1).

Figure 1. Change in the degree of metamorphism of groundwater in the Upper Jurassic deposits.

The diversity of waters with respect to chemical composition tends to decrease, as their salinity increases. The seven types allocated in water salinities ranging from 2 to 5 g/dm³ are distributed among the following groups: 10-15 g/dm³—five, at 20-25 g/dm³—two, with TDS value more than 25 g/dm³—only one (sodium chloride) type. The background salinity value for groundwaters of the upper Jurassic aquifer complex in the studied region averages 19.9 g/dm³. The area comprising the Severny (Northern) and Nizhnevartovsk arches, East Pur megamonocline and South Nadym megamonocline is characterized distribution of groundwaters with salinities exceeding 25 g/dm³. The highest values of the zonal hydrogeochemical background are accounted for the Severny arch structures where TDS of the background formation waters reaches 33.5 g/dm³.

Jurassic and Cretaceous paleohydrogeology and the existing paleohydrogeochical conditions of the study area are considered below in detail.

4. Results and Discussion
The periodization of hydrogeological history revealed three hydrological cycles in the Jurassic and Cretaceous: Induan-Sinemurian, Pliensbachian-Cenomanian, Turonian-Serravallian. Hydrogeological history of the sedimentary cover starts with the Induan-Sinemurian cycle. The onset of sedimentation is associated with the active volcanic activity and the formation of volcanic-sedimentary (Turin series) strata [17]. In the Triassic-Early Jurassic, Western Siberia was an uplifted, slightly dissected, gently elevated land area with the dominance of the processes of infiltration of fresh atmospheric water.

In the earliest Pliensbachian-Cenomanian hydrogeological cycle, the sea moved inland from the north-west and north-east. The marine basin was shallow (25 m) with desalinated water, while the Gydan and Yamal Peninsulas were represented by the shoal zone, where significant fluctuations of water salinity from 2 to 15 g/dm³ resulted from the unstable marine regime and river discharge. This is also corroborated by a paucity of the organic world (ammonites and brachiopods were not abundant, while pelecypods proved to be numerous, which is characteristic of the coastal areas), to some extent absorbed by clay complex (low K and Mg and high Na and Ca contents) [2, 18]. The southern part of the area was represented by a coastal plain, occasionally flooded by the sea and low-lying alluvial
plain located on the site of present-day Bolshaya Kheta megasyncline. Owing to the “mobility conditions” of the moving coastline there, coastal-marine and continental sediments were formed with the remains of leaf flora, plant detritus, accompanied by burial of predominantly Na Cl waters with high content HCO$_3^-$ and Ca$^{2+}$ and salinity values of 2-5 g/dm$^3$.

As the basin gradually shallowed in the southern direction, and the type of depositional settings changed, accordingly, from coastal-marine to continental (low-lying plain of accumulation), where processes of infiltration of fresh atmospheric water (from 0.5 to 2 g/dm$^3$) were predominant. The basin boards represented by themselves an elevated denudation plain, grading into the low-mountain relief (the Taimyr, Novaya Zemlya, Ural and Central Siberian uplands), acting as the provenance areas of clastic material and exterior source-areas of infiltration, within which Ca and HCO$_3^-$ waters salinity not exceeding 0.5 g/dm$^3$ were buried. The largest transgression of the sea basin over the time spanning the Early and Middle Jurassic is assigned to the Toarcian. The marine sedimentation zone has significantly extended within the study area, causing the basin deepening to a depth of 100 meters in the central part, with water salinity probably reaching 15-20 g/dm$^3$. This area encompassed the territory of the contemporary Kara, Antipayuta, Tadebeyakha and Bolshaya Kheta megasynclises and the Agapa- Yenisei trench. The fine-dispersed dark grey and black clayey silts accumulated in the deep-water part of the Kiterbyut Formation, which evolved into the source-rock. The finds of marine fauna (rostra of belemnites, bivalve, foraminifera) indicate the established normal marine sedimentation regime in the region [7].

The shallow-water area (< 25 m) rimmed the marine basin along its entire periphery. Less saline (2-15 g/dm$^3$) NaCl waters with elevated amounts of HCO$_3^-$ and Ca$^{2+}$ ions were buried within its limits, in parallel with the processes of sedimentation. The second half of the Toarcian – the beginning of Aalenian is characterized by short-term, but extensive regression of the boreal seas, which led to the shallowing and desalination of the West Siberian marine basin. The area of marine sedimentation (25-100 m) in the north-west has declined due to the expansion of the shallow (< 25 m) water zone. In the second half of Aalen, the climate gradually turned to cool and humid, causing vegetation to perish, along with the wide distribution of carbonaceous strata and the appearance of Arctic genera of ammonites and belemnites in the basin [18].

The beginning of Bajosian was marked by short-term sea-level rises leaving no significant impact on the position of the paleogeographic regions. Despite the fact that in the Bathonian, the subsidence of the Arctic regions of Western Siberia continued, the position of zones of marine sedimentation practically remained unchanged, however the periods of sea ingestion extended. In the north of the region, the extent of shoaling has increased due to the flooding of the low plain of accumulation rimming the basin boards. Callovian age is characterized by a continuation of the extensive marine transgression which resulted in further deepening of the marine basin occupying almost the entire area of the West Siberian geosynclise, except its southern margins. At that time, clayey beds of the Golchikha and Yakovlevka Formations accumulated in the deep-sea environments, which subsequently evolved into the regional seals. The sea depth in the most submerged part reached 400 m; the deep-water area located in the central part of the region encompassed the area of the present-day Kara and Antipayuta-Tadebeyakha megasynclises.

In this part of the marine basin, water salinity might reach 40 g/dm$^3$, which corresponds to average ocean salinity and is evidenced by the composition of authigenic minerals and a wide variety of fauna (bivalves, foraminifera, cephalopods and gastropods. This area was rimmed by shallower waters, where accumulated fine, substantially clayey sediments with layers of calcareous clays and glauconite with abundant fauna [18]. This portion of the basin is featured by salinity was in the range 20-30 g/dm$^3$ with the increasing role of Mg in the progressively buried seawater. A small area of the shoal zone with a sea depth up to 25 meters and up to 80 km in width, where developed different sediments facies and Na Cl waters with high concentration of HCO$_3^-$ and Ca$^{2+}$ ions and salinity in the range from 5 to 15 g/dm$^3$ were buried. Accordingly, the area of continental sedimentation zones has significantly reduced. At the turn of the Callovian and Oxfordian, the transgression was succeeded by regression which reached its maximum in the middle of Oxfordian. Given that the basin was shoaling, thick sand layers
began to accumulate in its central and southern parts, forming the known today Oxfordian regional reservoir. The northern areas were still dominated by the marine environments, providing for the formation of predominantly clayey sediments of the Golchikha Formation, rich in organic matter and containing abundant remains of diverse marine fauna. Since almost the entire study area was represented by a zone with depths between 25 and 200 m, salinity levels of the waters that experienced burial were, accordingly, close to 30 g/dm³ (figure 2). Given that the Jurassic transgression was the lengthiest event, the extent of the marine sedimentation have widened, and the depth in most of the area reached 200 m in the Late Oxfordian-Kimmeridgian time [7]. In the Volgian time (Tethonian-Early Berriasian) the dipping of the basin proceeded intensely, with the transgression reaching its maximum in the middle of the century. Climate in the Volgian was close to semiarid, causing thereby the dominance of chemical weathering conditions in the onshore areas and the accumulation of mainly clay and organogenic rocks on the continental shelf. In view of relief peneplanation, biogenic sedimentation was dominating, with clay sediments rich in organic matter, calcium, and silicon forming ubiquitously in the area (Bazhenov, Golchikha, Yanov Stan, Danilovka, Tutleima Formations) [18].

Figure 2. Paleohydrogeochemical map for the Oxfordian. 1 – the boundary of the Jurassic sedimentary basin; 2 – the boundary of paleohydrogeochemical zones: 3 – low mountains, the processes of infiltration of fresh meteorogenic waters with mineralization up to 0.5 g/dm³ and with the predominance of HCO₃⁻ and Ca²⁺ ions predominate; 3 – elevated plain, fresh and brackish inflitrogenic waters with a mineralization of 0.5-1.5 g/dm³ with predominance in the composition of HCO₃⁻ and Ca²⁺ ions with an increased content of Cl⁻ and Na⁺; 4 – denudation-accumulative plain, fresh and brackish inflitrogenic waters with a mineralization of 1.5-2.0 g/dm³ with predominance in the composition of HCO₃⁻ and Ca²⁺ ions with an increased content of Cl⁻ and Na⁺; 5 – low accumulative plain, burial of brackish water with mineralization 2-5 g / dm³ and predominance in the composition of Cl⁻ and Na⁺ ions of increased content of HCO₃⁻ and Ca²⁺; 6 – coastal plain, syngenetic brackish waters with a mineralization of 5-15 g/dm³ with a predominance in the Cl⁻ and Na⁺ ions with an increased content of Mg²⁺ and Ca²⁺ ions; 7 – shallow part of the shelf, coastal zone and island part of the shelf up to 25 m, saline thalassogenic waters with mineralization of 15.0-20.0 g/dm³ with a predominance of Cl⁻ and
Na⁺ ions with an increased content of Mg²⁺ ions; 8 – sea, 25-200 m, salty thalassogenic waters with mineralization 20.0-30.0 g/dm³ with a predominance of Cl⁻ and Na⁺ ions with an increased content of Mg²⁺ ions; 9 – deep sea 200-400 m, salty thalassogenic waters with salinity of 35.0 g/dm³ with a predominance in the Cl⁻ and Na⁺ ions with an increased content of Mg²⁺ ions.

Thus, by the end of the Volgian time, a deep basin with signs of hydrogen sulfide exposure had formed in Arctic region of Western Siberia. Almost the entire study area was flooded by the sea with depths of 200-400 m, where water salinity reached 35 g/dm³. In addition, two deep depressions were distinguished within the borders of the Kara and the Bolshaya Kheta megasynclises, where depths exceeded 400 meters, assumingly reaching 600 m where water salinity, hypothetically, could be 35 g/dm³. The zone was surrounded by a narrow strip of shallower part of the basin (100-200 m), where marine sedimentation was complexed with the burial of saline thalassogenic waters featured by salinity 20-30 g/dm³ and predominance of Cl⁻ and Na⁺ ions in the composition, and enhanced Mg²⁺ ion concentrations. Delineation of the coastal zones has practically not changed: the coastal plain was almost entirely flooded by the sea and marked only by small narrow strip along the eastern board of the basin, while the alluvial plain existed only in the coastal part adjacent to the Taimyr upland. The basin coasts became flatter and peneplenized, representing by themselves elevated denudation land area. In addition, a series of peninsulas was discriminated along the eastern board. The burial of fresh atmogenic, slightly saline Ca HCO₃ waters with salinity not exceeding 1-2 g/dm³ was taking place within the continental sedimentation zones.

A small in size deep-water zone was preserved in western Gydan Peninsula. Eastwardly, the shallow water area, which occupied almost half of the territory, has increased significantly. An extensive coastal plain formed in the south, where flood-plain, deltaic and beach depositional settings alternated depending on the sea level, and brackish waters with salinity 2-5 g/dm³, Na and Cl in composition, with high concentration of HCO₃⁻ and Ca²⁺ ions were buried. In the period spanning from the Barremian to the end of the Cenomanian, the study area was characterized by alternation of sedimentation conditions between low-lying accumulation plane and coastal plain (Kontorovich et al., 2014), where infiltration of meteoric Ca HCO₃ water with salinity from 0.5 to 2 g/dm³ were mixed with sedimentary waters in the area of active water exchange, partially diluting and desalinating them. Later transgression, which began in the Turonian period, resulted in the formation of a vast shoal zone, covering the entire study area through the Late Campanian. Salinity of sea waters could reach 15 g/dm³ in the deepest parts of the South-Western sea. In the Late Campanian, regression of the marine basin was accompanied by warming of the West Siberian sea, resulting in the deposition of calcareous sediments and causing an increase in the extent of the coastal plain. At this time, the composition of syngenetic waters was dominated by the infiltration-driven Ca HCO₃ with high concentration of Cl⁻ and Na⁺ ions and salinity reaching 2-5 g/dm³ in the coastal-continental environments. The following – Turonian-Serravallian – hydrogeological cycle commenced in the earliest Turonian. In Arctic regions of the West Siberian basin, shallow marine sedimentation conditions (up to 100 m) prevailed, the deepest part of the basin was situated in the western half of the study area. The shallow-water portion of the basin was rimmed by the low-lying accumulation and coastal plains from the east, and elevated – from the west. In the Late Campanian-Danish, the regression resulted in the marine basin shoaling (depth: < 25 m). Most of the region still comprises two shallow water zones, while a coastal plain, occasionally flooded by the sea developed within the eastern margin.

5. Conclusions

It follows from the above that the Jurassic-Cretaceous marine sedimentation regime dominated in Arctic regions of Western Siberia until the end of the Hauterivian and throughout almost entire Upper Cretaceous. Regular sea level fluctuations caused minor transgressions and regressions, the basin is found to have been the deepest in the Volgian time. The chemical composition of the Arctic basin bears no indications of any significant changes at the Triassic-Jurassic boundary. Systematic decreases were reported for potassium and sodium concentrations while the levels of calcium and magnesium
tended to increase. Driven by the basin deepening, a significant increase in salinity occurred at the turn of the Middle - Late Jurassic, and desalination – at the end of the Early Cretaceous. At that time, salinity of syngenetic waters might reach 35 g/dm³. A detailed analysis of modern hydrogeochemistry of petroleum-bearing deposits with account of paleohydrochemical reconstructions allowed to establish the dominance of sedimentary waters in the section, sometimes diluted by ancient infiltrates that penetrated during the marine basin regressions, which agrees well with the results of the paleogeographic constructions for the Jurassic and Cretaceous [7-8]. Local distribution was reported from condensate-prone waters of common origin with hydrocarbon accumulations. The "water-rock-gas-organic matter" system plays a critical role in the processes of the formation of chemical composition of groundwaters within petroleum-bearing deposits.

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