



# Hydrogeochemical classification of deep formation waters



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## ABSTRACT

Deep formation waters from Western Europe, Russia and North America are classified by the major water components ( $\text{Ca}^{2+}$ ,  $\text{Cl}^-$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ) and barium/sulphate ratios. The data are used to identify important hydrogeochemical processes (e.g., halite dissolution and albitisation) that lead to the different composition of formation waters. Two significant water types are identified: Na–Cl water and Na–Ca–Cl water. Furthermore, differences in formation water according to stratigraphical units are shown for deep reservoirs in the North German Basin and the North Sea. Based on the collected hydrogeochemical data, development trends are stated for the formation waters, and albitisation is favoured as the main process causing Ca enrichment.

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## 1. Introduction

There are several terms to describe deep fluids of the Earth's crust. Kharaka and Hanor (2007) list the following descriptions: oil-field brine, basinal brine, basinal water, and formation water. In our paper we decided to use the term “deep formation water”, because we focus on groundwater from deep formations in all kinds of geological units. The term brine refers to water salinity higher than 5%, but not all formation waters reach this salinity level.

Anthropogenic activities (e.g., shale gas extraction,  $\text{CO}_2$  sequestration, geothermal energy production and deep waste disposal) can change the hydrogeochemical characteristics of deep formation water. To predict such changes, the natural processes in deep reservoirs should be known and the influence of anthropogenic impact should be evaluated.

Formation water in deep sedimentary basins can be classified according to depth, temperature, and salinity (e.g., Graf et al., 1966; Kharaka and Hanor, 2007). Most of the deep formation waters contain more dissolved solids than seawater and are unsuitable as human drinking water. The hydrogeochemical development of formation water has been discussed for a long time. It is widely accepted that deep aquifers are influenced by the meteoric water cycle and geochemical processes within the crust (Hebig et al., 2012). Similar hydrogeochemical signatures are found in deep formation waters on all continents and can be explained by

general geochemical processes within the deep reservoirs (Land, 1995). The main hydrogeochemical processes that are thought to be responsible for the hydrochemical composition of deep formation waters are:

### 1. Seawater evaporation

This process has been thoroughly investigated (e.g., Usiglio, 1849; Clarke, 1924). The steps in evaporation that lead to different brine compositions and mineral precipitations are understood and can be retraced through modelling (e.g., Eugster et al., 1980). Recently formed brines resulting from seawater evaporation can be observed in dry areas (e.g., Dead Sea, Kara Bogas Gol) and in salt mines (Fontes and Mantray, 1993a). Several authors have discussed seawater evaporation as a process leading to the composition of deep formation water (e.g., Lowenstein et al., 2003; Lowenstein and Timofeeff, 2008; Houston et al., 2011). Lowenstein and Timofeeff (2008) favour residual brines as the main contributor to deep formation water and also suggest that changes in the chemistry of ocean water (especially  $\text{Ca}^{2+}/\text{SO}_4^{2-}$  ratios) can be responsible for the development of brines dominated by calcium chloride. Residual evaporation brines dominated by magnesium, sulphate and chloride seem to be only occasionally present in deep reservoirs (Tesmer et al., 2007).

### 2. Salt dissolution

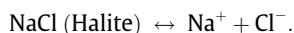
The dissolution of salt layers and salt domes will increase the salt concentration of meteoric and surface groundwater that is in contact with the salt deposits. Halite is the dominant precipitated

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salt in most geological units, and therefore halite will be dissolved, and halite dissolution leads mainly to the enrichment of sodium and chloride in deep formation waters. Mass balance scenarios considering the interaction of formation water with crustal rocks (Land, 1995) validate the conclusion that evaporites must have been deposited and destroyed at much greater rates during geological history than existing salt inventories suggest.

The dissociation of halite is chemically described as:

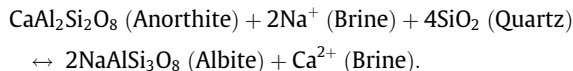


The amount of dissolved halite increases with rising temperature.

Bromide is another indicator for the dissolution of halite deposits (e.g., Land and Prezbindowski, 1981; Walter et al., 1990). Bromide cannot be included in the crystal lattice of halite, because of its larger ionic radius, therefore it enriches the residual solution during seawater evaporation. Formation water derived from the dissolution of halite will have the chloride/bromide ratio of halite. This leaching induces low bromide concentration, and the chloride/bromide ratio resulting from halite dissolution is much higher than the ratio developed during seawater evaporation.

### 3. Feldspar transformation

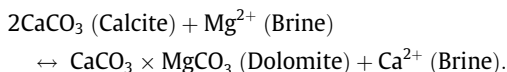
During this process  $\text{Ca}^{2+}$  ions are added to deep formation waters. The transformation of different feldspar minerals has been discussed already over many years (e.g., Davisson and Criss, 1996; Houston et al., 2011; Land, 1995; Pinneker, 1966; Spencer, 1987; Tesmer et al., 2007). Special focus has been given to the albitisation of anorthite in Na–Cl dominated brines summarised by the following reaction:



According to thermodynamic equilibrium conditions, this reaction favours Ca enrichment of formation waters.

### 4. Dolomitisation

The term dolomitisation refers to the replacement of calcite by dolomite. Dolomitisation is often explained as a reaction between brines and calcite. It leads to a loss of Mg as dolomite is formed and is summarised by the following chemical reaction:



The opposite process, dedolomitisation, caused by Ca-rich brines can also change the formation water composition and lead to an enrichment of Mg (Land and Prezbindowski, 1981; Stoessell et al., 1987).

There are several conceptual models for dolomitisation that Gasparrini (2003) has split into three main groups: evaporate and seepage-reflux models, fresh and seawater mixing models, and burial (subsurface) models. Machel (2004) argues for the use of the term dolomitisation only when  $\text{CaMg}(\text{CO}_3)_2$  replaces  $\text{CaCO}_3$ , and not for the primary precipitation of dolomite.

Further processes that are thought to influence deep formation water are membrane filtration or osmosis in clay layers, shales and siltstones (e.g., Graf, 1982; Hitchon et al., 1971; Kharaka and Hanor, 2007), diffusion (e.g., Ranganathan and Hanor, 1987), and freezing of saline water (e.g., Herut et al., 1990). The solubility of calcite at different temperatures and pressures has been well investigated (e.g., Coto et al., 2012; Duan and Li, 2008). Even considering the high  $\text{CO}_2$  pressures within deep formations, calcite solubility does not induce the high Ca concentrations found in most formation waters, whereas the portion of  $\text{HCO}_3^-$  concentrations can be attributed to calcite solubility (Lehmann, 1974). Often the origin of the salt contents in groundwater cannot be explained by just one process. The saline groundwater of the Canadian Shield, for example, where no salt layers are found, is attributed to the inflow of brines from other strata, the leaching of salt from fluid inclusions and special mineral reactions (Frape and Fritz, 1987).

**Table 1**  
Short characteristics of regions from which geochemical data were used for this study (occurrence of salt layers: from large deposits “+++” up to minor deposits “+” and no salt deposits “–”).

| Region                           | Geological units from which water was mainly sampled | Presence of evaporite layers  | Reference  |
|----------------------------------|--|---|--|
| <i>Western and Middle Europe</i> |  |   |  |
| North German Basin               | Carboniferous – Tertiary                             | +++ (Permian, Triassic) Permian salt domes often reach up to the surface. | Hesshaus et al. (2013)<br>Kühn et al. (1998)<br>Lüders et al. (2010)<br>Regensburg et al. (2010)<br>Schulz and GeotIS-Team (2009)<br>Warren and Smalley (1994) |
| North Sea                        | Devonian – Eocene                                    | +++ (Permian, Triassic) Permian salt domes often reach up to the surface. |  |
| Paris Basin                      | Triassic – Tertiary                                  | ++ (Triassic: Muschelkalk and Keuper)                                     | Fontes and Mantray (1993b)   |
| <i>Russia</i>                    |  |   |  |
| Southwest Ural                   | Cambrian – Permian                                   | ++ (Cambrian, Devonian, Permian)  | Nosareva (2007)  |
| Siberia                          | 1. Precambrian – Ordovician                          | 1. ++ (Cambrian)  | Shouakar-Stash et al. (2007)   |
| 1. Angara Lena Basin             | 2. Precambrian – Permian                             | 2. ++   |  |
| 2. Tunguska Basin                | 3. Cambrian – Tertiary                               | 3. ++   |  |
| 3. Yakutian Basin                | 4. Precambrian – Silurian                            | 4. –  |  |
| 4. Olenek Basin                  |  |   |  |
| Angara Lena Basin <sup>a</sup>   | Precambrian – Ordovician                             | ++ (Cambrian halite–carbonate deposits: 3000–4000 m thickness)            | Pinneker (1966)  |
| <i>America</i>                   |  |   |  |
| Canadian Shield                  | Precambrian (crystalline rocks)                      | –   | Frape and Fritz (1987)   |
| Western Canada (Alberta)         | Devonian – Cretaceous                                | ++ (Devonian)   | Hitchon et al. (1971)  |
| Illinois Basin                   | Silurian – Devonian                                  | + (Gypsum and anhydrite)  | Stueber and Walter (1991)  |
| Palo Duro Basin                  | Carboniferous – Triassic                             | +++   | Knauth (1988)  |
| Mississippi Salt Dome Basin      | Jurassic – Cretaceous                                | +++   | Kharaka et al. (1987)  |
| Texas Gulf Coast                 | Jurassic – Miocene                                   | +++   | Kharaka et al. (1977)  |
| Gulf of Mexico                   | Jurassic – Miocene                                   | +++ (Jurassic)  | Houston et al. (2011)  |

<sup>a</sup> The dataset of Pinneker differs from the data given in Shouakar-Stash et al. (2007).

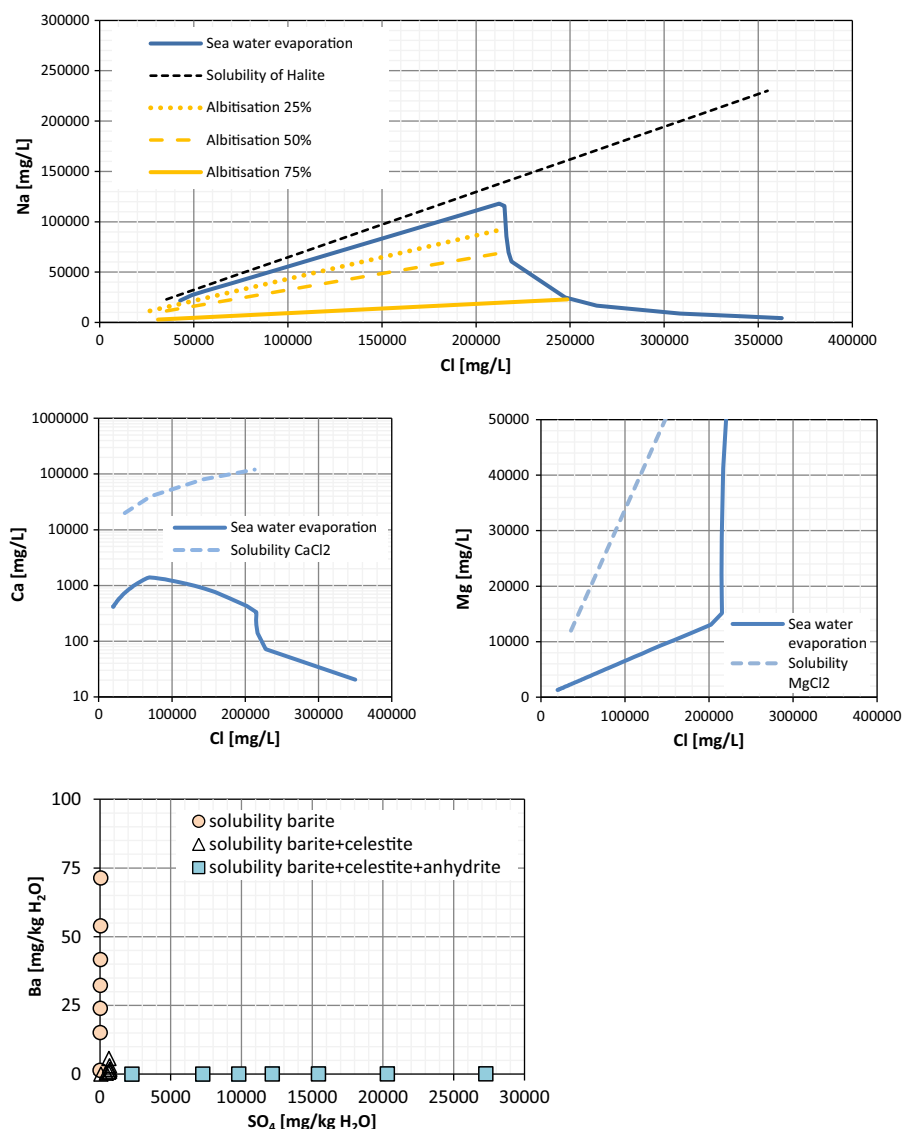
Any investigation of the hydrology and geochemistry of formation waters must be based upon paleohydrological studies, including information concerning sedimentology, stratigraphy, diagenesis and geology (Kyser and Hiatt, 2003). Within the crust and in accordance with a long residence time, all types of formation water can be affected by mixing processes. Even mixing with recent meteoric water cannot be excluded. Tesmer et al. (2007) present mixing models of evaporated modern seawater and brines from different evaporation steps (the beginning of sylvite, carnallite and bischofite crystallisation). The chemical composition of German formation waters can be retraced using such mixing models, but the geological conditions including regional fault systems as pathways for such mixing processes and the connection of the recent deep formations to the meteoric cycle in former times are not discussed by the authors. Considering the volume of deep formation water, such a mixing of residual brines with seawater also seems to be problematic.

In this study, the hydrogeochemical signatures of deep formation waters from Western Europe, the Russian and Siberian platform, and North American basins and shields (Table 1) are compared and classified.

## 2. Methods

The collected data of formation waters (Table 1) were analysed, and the main ions that can be used to classify water types were identified. The content of Total Dissolved Solids (TDS) was calculated by adding the main ions and compared to the given data. Where the differences between the calculated and the given TDS content could not be explained (e.g., by the correction of simple mistakes seen in ionic balances), the concerned data were not used in further data assessment. Sampling methods for deep formation waters are not evaluated in this study. The question of whether chemical equilibrium is reached during the sampling is also not discussed.

The data were inserted into different diagrams. To facilitate data interpretation, the diagrams were completed with graphs showing typical geochemical processes within deep reservoirs (seawater evaporation, halite dissolution, and feldspar transformation), which are already discussed in Chapter 1. Barite solubility is also considered. Seawater evaporation data were calculated using the code PHREEQC (Parkhurst and Appelo, 1999) in combination with the database “pitzer.dat”. The starting solution has a contemporary seawater composition. The evaporation process is modelled



**Fig. 1.** Chemical processes (seawater evaporation, solubility degree of NaCl (halite),  $\text{CaCl}_2$ ,  $\text{MgCl}_2$ , steps of albitisation, barite solubility) indicated by ratios of Na/Cl, Ca/Cl, Mg/Cl, and Ba/SO<sub>4</sub>.

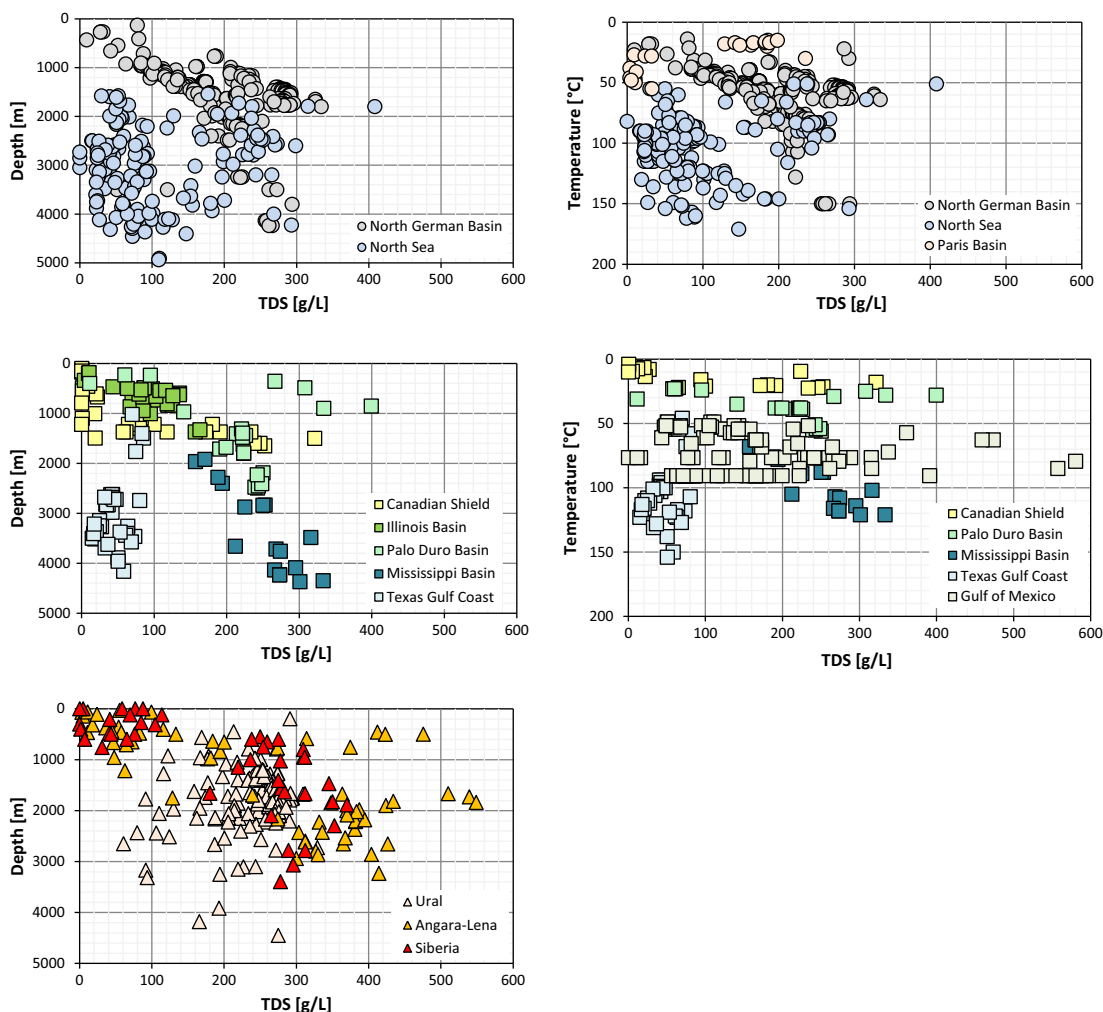


Fig. 2. TDS, temperature vs. depth of formation waters from Western Europe, Russia and North America.

via the order “reaction” by a stepwise increasing subtraction of water. Halite precipitation starts at a chloride concentration of about 210 g/L and is clearly seen in decreasing sodium and calcium concentrations, and rising magnesium concentrations in the diagrams.

The line representing halite dissolution follows the dissociation reaction up to maximal solubility of ca. 6 m halite at 25 °C. Higher molalities (up to 10 m) of dissolved halite are reached with rising temperatures. The same procedure was used to draw the solubility line of  $\text{CaCl}_2$  (mineral: antarcticite  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$ ) and  $\text{MgCl}_2$  (mineral: bischofite  $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ ). Feldspar transformation (albitisation) was considered in several steps (25%, 50%, and 75%) for solutions with different sodium concentrations. For the graphs of the diagrams this process was simply calculated by subtracting  $\text{Na}^+$  ions and adding  $\text{Ca}^{2+}$  ions to the solution keeping the stoichiometric ratio 2:1 (charged balanced Na/Ca exchange). Feldspar transformation exceeds the solubility of antarcticite because this mineral is relatively seldom found in the lithosphere.

To compare the measured barium and sulphate concentrations with the concentrations resulting from the solubility of barite only and barite solubility in the presence of celestite ( $\text{SrSO}_4$ ) and anhydrite ( $\text{CaSO}_4$ ) in 0–6 m NaCl solutions, these solubilities at 25 °C are calculated by modelling. The code PHREEQC is used, in combination with the “gebo” database (Bozau, 2013) that was specifically developed for the hydrogeochemical modelling of deep formation water in the North German Basin. The “gebo” database provides additional thermodynamic data for the Pitzer database, which is

delivered with the code PHREEQC, and was successfully tested for barite solubility in NaCl solutions (Bozau, 2013). The rising molality of the NaCl solution leads to increasing solubilities of sulphate minerals, in accordance with the “salting in” effect (Blount, 1977).

The graphs indicating all considered geochemical processes are shown in Fig. 1. Although the sampling depth and temperature are not given for all the collected chemical analyses, diagrams considering depth, temperature and TDS contents were also drawn up (Fig. 2). The main components (Ca, Cl, Mg, Na) for all study areas are plotted in Fig. 3. The barium and sulphate ratio for study areas in Western Europe and North America is shown in Fig. 4. The barium concentrations of the Russian samples are not given. Stratigraphical data from the North German Basin and the North Sea allow for a further classification: water chemistry vs. geological unit shown in Fig. 5.

### 3. Results and discussion

Despite differing regional geological development, the formation waters of various regions are compared by their depth, temperature and chemical composition (TDS and elemental ratios). More features concerning the geological setting of the study areas are given in the references cited in Table 1. Geology and tectonic characteristics are specific in all considered regions and do not draw on a simple worldwide classification of deep formation

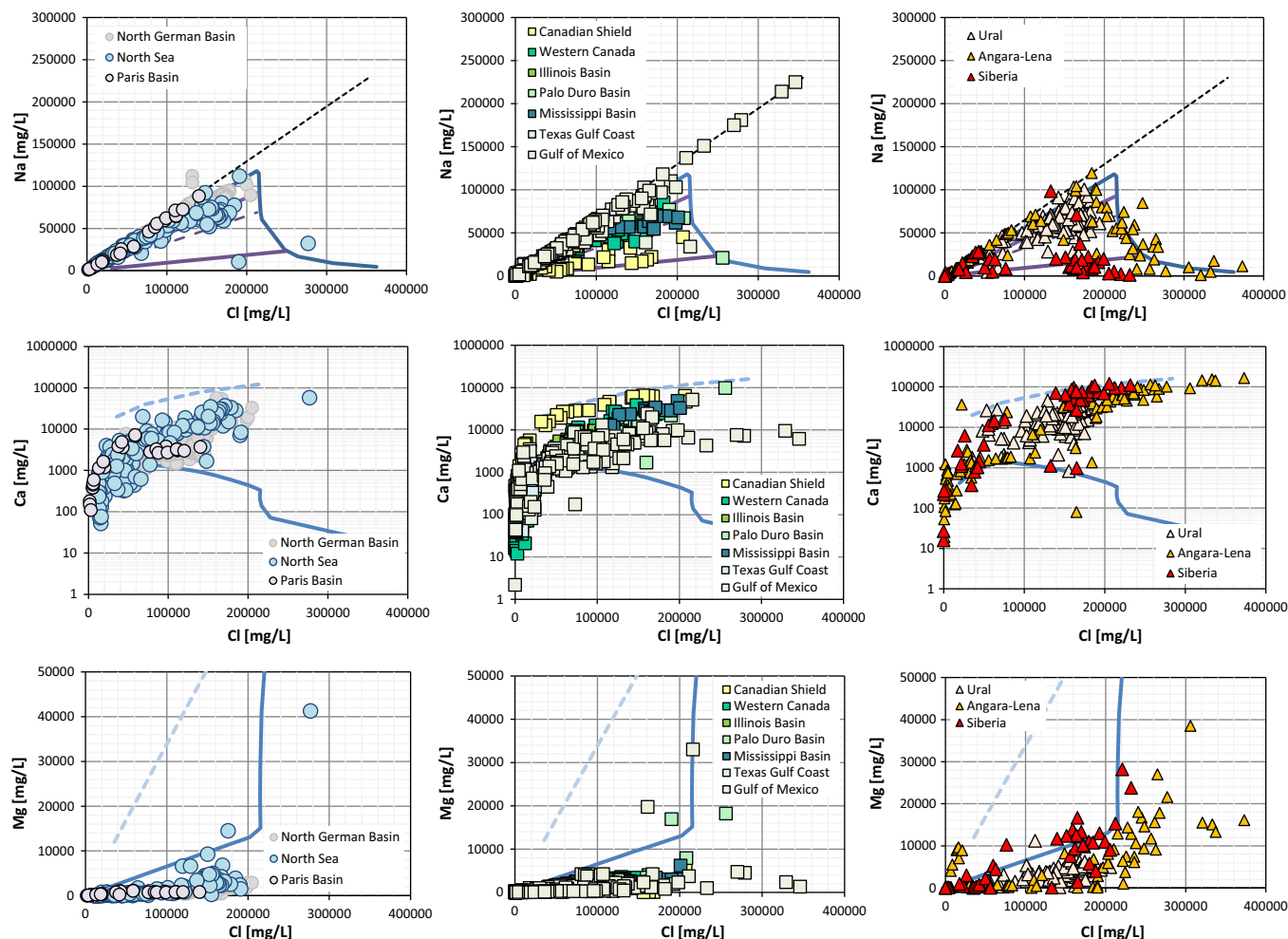


Fig. 3. Na, Ca, Mg vs. Cl of formation waters from Western Europe, Russia and North America.

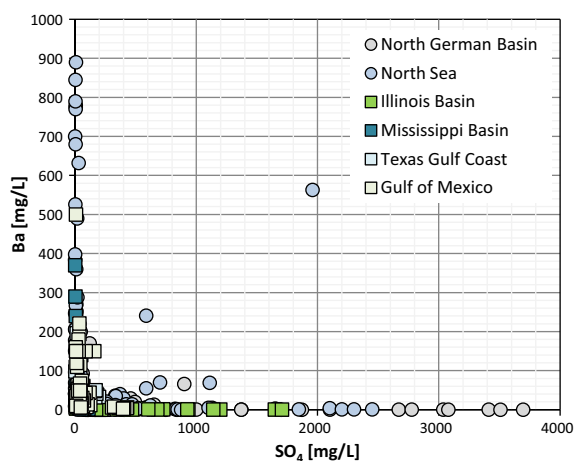


Fig. 4. Ba vs.  $\text{SO}_4$  of formation waters from Western Europe and North America.

waters. There are many differences in the geological development of basins and shields. Furthermore, drill holes in basins with continuous sedimentation and sedimentary rocks will reach greater depths than drill holes on shields consisting of older sedimentary and igneous or metamorphic rocks. The present classification focuses only on hydrogeochemical signatures, however, and

therefore, this study does not involve a detailed geological interpretation.

Generally, the mineralisation of formation water indicated as TDS content is rising with depth and increasing temperature in all study areas (Fig. 2). This trend is clearly seen for the North German Basin, the Mississippi Basin, the Illinois Basin and most of the Russian samples. Exceptions are the data from the North Sea and the Gulf of Mexico, as well as some data from the basin SW of the Ural Mountains. Formation water with TDS contents of lower than 100 g/L is sampled in depths from 1000 m up to 5000 m in these areas.

The majority of samples reaches TDS contents of about 400 g/L. TDS contents higher than 400 g/L are only found in one sample from the North Sea, four samples from the Gulf of Mexico and eleven samples from the Angara-Lena Basin. The highest TDS content in the North Sea with a calculated amount of 408 g/L is found in the Permian layers of Leman Field. It is the only Zechstein water of this dataset that is characterised as Ca–Mg–Cl water. Angara-Lena waters with TDS contents of more than 300 g/L are described as very strong brines and Ca–Na/Mg–Cl waters. The waters with TDS contents higher than 500 g/L from the Angara-Lena Basin are also dominated by calcium and are found in the Cambrian salt layers. They are described as almost saturated brines by Pinneker (1966). The main anion of the highly mineralised samples from the Gulf of Mexico is sodium. These samples are related to relatively low reservoir temperatures and represent other formation processes (dissolution of halite), in comparison with the highly



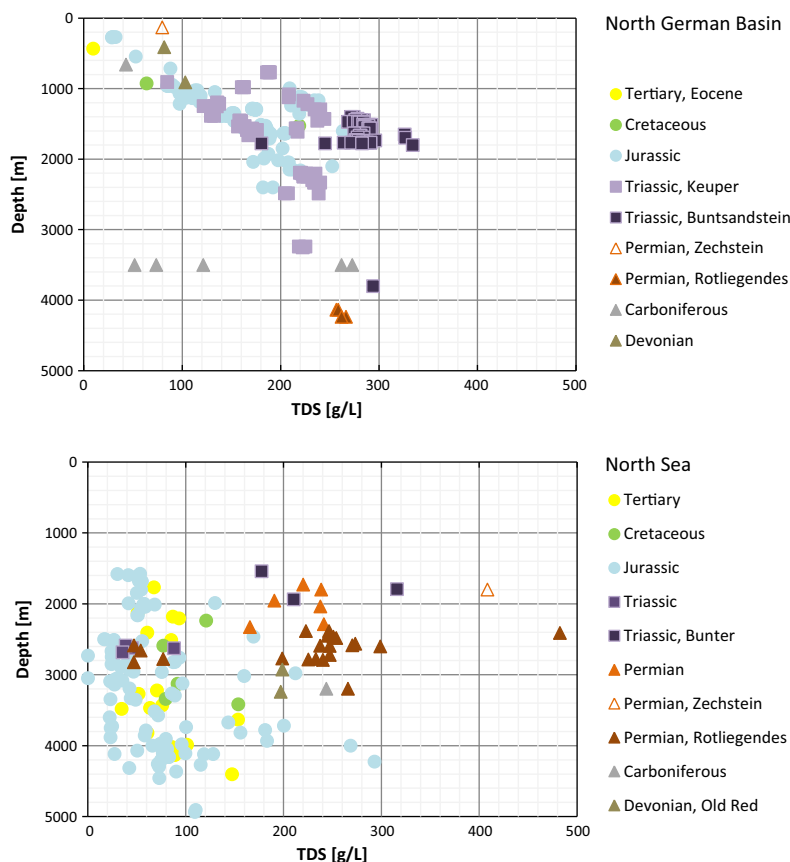


Fig. 5. TDS vs. depth of formation waters in the North German Basin and the North Sea.

mineralised waters from the North Sea and the Angara-Lena Basin, where some residual brines can be found, and intensive water–rock interactions must have led to the enrichment of Ca in most of the samples. Figs. 1 and 3 show the main processes leading to the chemical composition of deep formation waters. Seawater evaporation, NaCl (halite), CaCl<sub>2</sub>, and MgCl<sub>2</sub> dissolution are indicated using graphs. Several steps of albitisation changing the Cl/Na ratio are also given. Furthermore, modelled barite solubility in combination with celestite and anhydrite solubility in different NaCl solutions (0–6 m) is shown in Figs. 1 and 4.

Salt deposits are found in all parts of the world and are developed in several geological units. In Western Europe, Permian salt deposits are dominant in the North German Basin and the North Sea (especially in the southern part of the North Sea). Triassic salts are found in the Paris Basin, the North German Basin and the North Sea. Even in the salt free rocks of the Canadian Shield, highly mineralised formation waters are found. Table 1 gives further information and indicates salt deposits in the investigated study areas. In accordance with seawater evaporation and the relatively constant composition of the ocean since Paleozoic times, the mineral composition of salt deposits is comparable all over the world. The main amount of deposited salts consists of halite.

The plotted formation water data (Fig. 3) indicate two main water types: Na–Cl waters and Ca–Na–Cl waters. These waters also represent the two main geochemical processes in formation water development: halite dissolution within sedimentary basins and feldspar transformation. Halite dissolution is mainly responsible for an increase in Na and Cl, whereas feldspar transformation and dolomitisation add Ca to the solution. The main anion of deep formation water is chloride. The majority of samples displays chloride concentrations up to 300 g/L. Sulphate concentrations in

formation waters (<10 g/L) are much lower than the chloride concentrations and can be explained by the solubility of sulphate minerals, mainly CaSO<sub>4</sub> (Lehmann, 1974). Due to the anoxic state of most of the deep reservoirs, sulphate reduction processes will lower the sulphate concentration within the formation waters. Hydrogen carbonate concentrations are lower than sulphate concentrations (up to 2 g/L) and can be explained by the solubility of carbonate minerals such as calcite and dolomite in deep reservoirs (Lehmann, 1974).

Halite dissolution leads to a molar Cl/Na ratio of about 1. The low Br concentrations of Na–Cl waters also consolidate the conclusion that halite dissolution exceeds seawater evaporation processes within basins. During seawater evaporation Br increases in the brine and the precipitated halite has a very low Br content. Feldspar transformation, especially the formation of albite by dissolution of anorthite in the presence of quartz within NaCl solution, is considered to be the main process causing Ca enrichment in deep formation water. There is no Ca enriched salt mineral that allows for the extent of the Ca found within formation waters. Furthermore, NaCl solutions are much more abundant than MgCl<sub>2</sub> solutions, which are a prerequisite for dolomitisation. The collected data show that Mg, Cl and sulphate dominated waters (the end members of seawater evaporation) are rarely found in deep reservoirs. There are only a few formation waters with Mg concentrations higher than 10 g/L and Cl concentrations higher than 200 g/L. The highly concentrated samples of the Angara-Lena Basin are dominated by the cation Ca (up to 167 g/L) combined with Mg concentrations up to 38 g/L and K concentrations up to 21 g/L. They display relatively low Na concentrations. Fontes and Mantray (1993a) present one brine sample directly associated with Triassic salts in the Paris Basin where the Mg concentration (56 g/L) exceeds the Na concentration (38 g/L). Comparable concentrations

are found in the Dead Sea. Water from the Dead Sea (Oren and Ventosa, 1999), as the classic example of seawater evaporation, has a Mg concentration of 45 g/L and a Na concentration of 37 g/L. Furthermore, dedolomitisation can cause Mg enrichments. Increasing Mg concentrations could also be attributed to mafic and metamorphic rocks, as discussed for the deepest waters in the deep drill hole “Kola” (Nurmi et al., 1988).

Barite solubility increases with depth and with the TDS content of the water (Blount, 1977). Barium concentrations are often considered to be derived by barite solubility. Due to the common ion effect, Ba concentrations decrease when sulphate from the dissolution of celestite and anhydrite is released (Fig. 2). Ba concentrations can rise, however, by sulphate reduction that is often observed under anoxic conditions in deep reservoirs. The measured barium (up to 1000 mg/L) and sulphate concentrations (up to 4000 mg/L) display the modelled trend of lowering barium by increasing sulphate concentrations (Figs. 2 and 4). Differences between the highest modelled barium concentration of about 75 mg/L and the measured concentrations can be explained by sulphate reduction leading to a further increase of barite solubility and/or additional sources of Ba within deep reservoirs (e.g., feldspar and clay minerals). Differences between modelled and measured sulphate concentrations are attributed to bacterial or thermochemical sulphate reduction processes.

The relationship between depth and TDS content for the different geological units of the North German Basin and the North Sea are shown in Fig. 5. The general trend of TDS rising with depth in the North German Basin has not been found in the North Sea. The study areas seem to be not really comparable. Warren and Smalley (1994) differentiate between three geological zones within the North Sea: the Northern, the Central, and the Southern North Sea Province. Permian salts are absent in the Northern North Sea Province where no stratigraphical control on salinity is found and relatively low salinities (generally less than 70 g TDS/L) are measured in the formation water of Jurassic units. Waters from the Central North Sea Province, which range from Devonian to Eocene sandstones are more heterogeneous with TDS contents from 10 g/L to 350 g/L. At TDS contents of about 200 g/L, the sodium concentration of these waters remains constant and calcium concentrations rise. Warren and Smalley (1994) found no clear trends in the formation water of the Southern North Sea Province (mainly Permian Rotliegendes and Triassic Bunter sandstone) with salinities in excess of 100 g/L.

Therefore, water samples from the North German Basin should be stratigraphically compared with samples from the Southern and the Central North Sea Province. But unfortunately, there are no samples from the formation waters of the Upper Triassic sandstone (Keuper) of the North Sea Provinces. In the North German Basin, clear differences between Upper and Lower Triassic formation waters are seen. Most Permian and Lower Triassic samples from the North German Basin are characterised by TDS contents higher than 250 g/L and an enrichment of Ca. Waters of younger geological formations are dominated by Na and Cl. Such a trend is also seen by Warren and Smalley (1994) in the Central North Sea Province where it started with a TDS content of about 200 g/L. These data (especially the change of Na–Cl and Na–Ca–Cl water) from the North German Basin and the Central North Sea Province suggest that a stratigraphically based interpretation seems to be possible. To confirm this thesis, further research must concentrate on detailed geological and geochemical information of the respective deep reservoirs.

#### 4. Conclusions

Deep formation waters from different geological units from all over the world can be divided into two main categories: Na–Cl

and Na–Ca–Cl waters. More than 95% of the investigated formation waters have TDS contents up to 250 g/L. Na–Cl waters mainly display TDS contents lower than 250 g/L. At TDS contents of about 250 g/L, Na–Ca–Cl waters are dominant in most of the investigated areas. The main anion of deep formation water is chloride in combination with the cations sodium (up to 120 g/L), calcium (up to 100 g/L) and magnesium (up to 10 g/L). Residual brines resulting from seawater evaporation and dominated by Mg and/or K with TDS contents higher than 300 g/L are rare.

Similar trends (increasing mineralisation with depth and temperature) are seen in most of the datasets from all the investigated regions. The main processes that lead to the composition of formation waters are salt dissolution and an enrichment of Ca by albitisation or dolomitisation. Considering the investigated data, MgCl<sub>2</sub> dominated formation waters as prerequisite for dolomitisation are rare. According to the preferential occurrence of NaCl dominated formation water, Ca enrichment by albitisation is supposed to exceed an enrichment of Ca caused by dolomitisation.

The main ions (Ca<sup>2+</sup>, Cl<sup>−</sup>, Mg<sup>2+</sup>, Na<sup>+</sup>) investigated in this study allow for a first description and classification of formation waters. But further chemical measurements will facilitate better understanding of the reservoirs and the development of the formation waters. Water rock interactions can be evaluated by REE concentrations and patterns or strontium isotope ratios. Isotope data (e.g., <sup>14</sup>C, <sup>δ</sup><sup>18</sup>O) and anthropogenic tracers are also helpful in calculating the residence times of formation waters or the contribution from the meteoric water cycle. Aqueous SiO<sub>2</sub> concentrations in combination with hydrogeochemical modelling for a correct calculation of activity coefficients can be used to estimate temperature in highly mineralised formation water.

Due to the heterogeneity of the Earth's crust, the complexity of rock composition, geochemical reactions and possible chemical changes induced by the technical equipment (well casing materials, pumping systems), the interpretation of hydrogeochemical data and the application of hydrogeochemical models for deep reservoirs should be carefully evaluated.

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