Chapter 1. Introduction

1.1 The North East German Basin: an unexplained large-scale transport system of dissolved halite

Solute and heat transport in aquifers are studied for their relevance in socio-ecological issues such as energy self-sufficiency and pollution of the environment. An example is the migration of dissolved halite released by salt structures which are commonly found in many geological formations. Subsurface dissolution of salt diapirs is usually invoked to account for the origin of saline groundwater in sedimentary basins (Posey and Kyle 1988; Musgrove and Banner 1993). Eventually, in some discharge areas, these saline waters reach the surface. Several mechanisms may be responsible for driving the heavier saline water up to the surface.

In the last decade, many studies, based on geothermal systems have demonstrated that temperature effects on liquid density can induce convective flows driving different dissolved solutes over long distances. Double-diffusive convection (DDC) is mentioned when the density variations are caused by two factors which have different rates of diffusion. The archetypal example is heat and dissolved salt in water, often referred to as thermohaline convection. In sedimentary basins, many situations in which fluid density varies occur because of changes in salt concentration, temperature and pressure of the groundwater (Cheng 1978; Oldenburg and Pruess 1998; Hanano 1998; Nield and Bejan 1999). Among the multitude of important environmental processes, the transport of pollutants released from waste disposal in salt rock formation (Evans 1989; Van der Lee 2001), saltwater intrusion in exploited costal aquifers (Kohout 1965; Reese 2003) or salt layers embedded in aquifers (Sarkar et al. 1995) can be mentioned. In all these cases, it is proved that density-driven convection can lead to transport of heat and dissolved salt over large spatial scales and significantly shorter migration time scales than compared with diffusion alone (Straus and Schubert 1977; Straus 1979; Hanor 1987; Simmons et al. 2001; Flocks et al. 2001; Diersch and Kolditz 2002; Simms and Garven 2004). Thermohaline convection in geothermal systems usually occurs together with regional-scale groundwater flow induced by topographic variation. The convective flow regime is then referred to as mixed convection. For instance, in Garven et al. (2001) mixed convection is investigated as a mechanism for deep fluid migration of base metal ores in the McArthur Basin, Australia.

An interesting example of deep fluid flow involving the mentioned processes of halite transport in a geothermal system is provided by the North East German Basin (NEGB). Here the NEGB environmental issues will be briefly introduced.

The NEGB is shown in Fig.1-1. Its area extends over of 330 km x 230 km in the North-South and West-East direction respectively. In different regions of the basin, brackish water reaches the surface locally. This phenomenon is manifested through the occurrence of salty springs or pots. A common characteristic of these saline springs is their temporary and spatially instability. Fig.1-1 illustrates the location of the known saline springs observed in the NEGB (Schirrmeister 1996) together with the distribution of saline groundwater occurring at shallow levels between 0 and 300 m (Grube et al. 2000). The northern and southern basin margins are also depicted. These dashed areas delimit the eroded sediments regions within the study area (denoted as "uplifted").

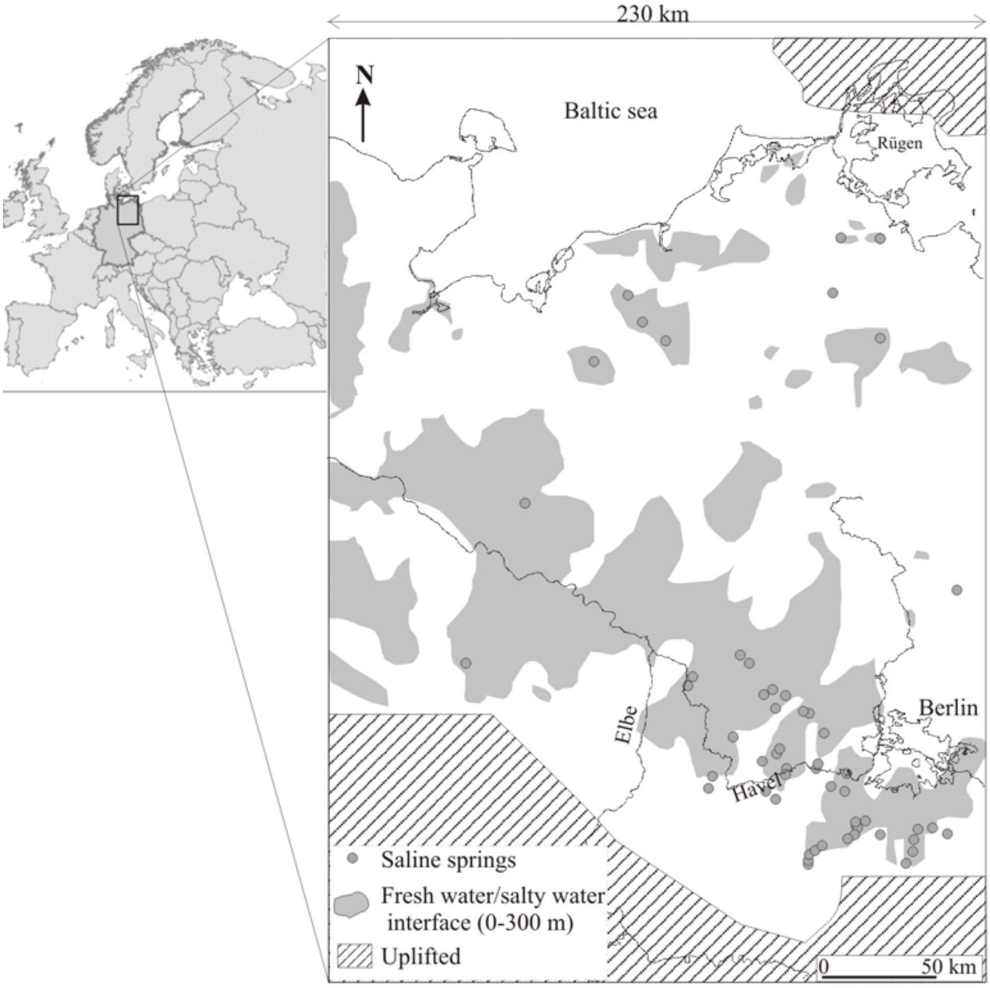

Fig.1-1: Study area, location of the observed springs (Schirrmeister 1996) and salty groundwater interface (Grube et al. 2000). The thin sediments area is denoted with "Uplifted".

From Fig.1-1 it can be seen that the main brine plume of saline groundwater slants across the basin stretching over 250 km from the western part to the south-eastern area near Berlin. In addition, isolated brine formations with an extension in the order of 20 km can be observed in the northern and western part of the domain. The discharge area of brackish waters occurs in the south-eastern part of the NEGB. Presently, the majority of the saline springs are observed in the neighbourhood of the Elbe and Havel rivers and to the south of Berlin. Only few of them are encountered far from these locations.

Further evidence of saline waters is given by plants commonly found along sea beaches or in salty soils, such as seashore salt grass, which grow in different areas of the basin. Fig.1-2 illustrates two species of these plants which have been photographed during a field trip in 2004 in Gröben, 50 km south of Berlin. The spontaneous growth of seashore grass far from the Baltic Sea coast is unusual and signals the existence of highly salty soils in the inner part of the basin.

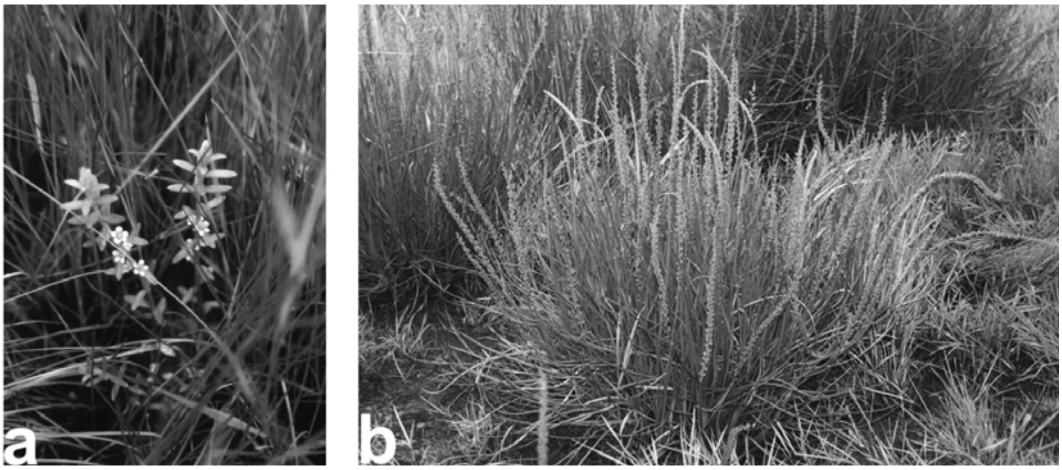

Fig.1-2: **a)** Glaux maritima (Sea Milkwort, Strand-Milchkraut) and **b)** Triglochin maritimum (Sea Arrowgrass, Strand-Dreizack). The pictures were taken during a field trip in Gröben in 2004.

Although these phenomena are observed since two centuries, the origin and mechanisms driving salt in the NEGB aquifer are not fully understood. Heck (1932) listed various locations of saltwater occurrences in Schleswig-Holstein which cannot be related to any shallow salt deposits or salt domes and whose cause remains unknown. A lack of explanation is also noted by Johannsen (1980) for steep vertical plumes of saline fluids reaching near-surface levels in Schleswig-Holstein that.

An important feature of groundwater flow systems within sedimentary basins is that hydrological, thermal and chemical mass transfer are closely coupled. As Chen et al. (1990, p.104) notes, “ Although we tend to think of a single process, it often happens that a variety of processes are coupled so strongly that qualitatively new effects and system behaviours arise because of this coupling”. Numerical modelling represents a powerful investigation tool which can provide new insights into basin fluid dynamics resulting from the strongly coupled transport processes. For instance, previous coupled heat and fluid transport simulations based on the NEGB (Clausnitzer et al. 2001; Bayer et al. 2002) suggested that the thermal anomalies, due to the presence of salt domes in the basin, may force local up-welling of deep-seated water in specific locations. However, this hypothesis needs further testing by recognizing salt effects on fluid density that were ignored in the models.

Therefore the main goal of the thesis will be to numerically investigate thermohaline convective flows in the NEGB in order to provide fundamental informations on the unknown mechanisms that lift deep salty groundwater to near-surface.

1.2 Data: aquifer and fluid model

Large scale simulation of coupled fluid flow, mass and heat transport based on real geothermal system requires a proper aquifer and fluid model. This is necessary because of the high spatial variability of the physical and chemical properties of the geological strata and the fluid. Therefore the input database must include:

- spatial aquifer characteristics (“aquifer model”), i.e. layer geometry, lithologies, and physical parameters of the different aquifers such as porosities, permeabilities, heat conductivity and heat capacity,
- chemical and physical fluid characteristics and their spatial distribution (“fluid-model”), i.e. water salinity, chemical components and fluid density.

In order to supply these input data, an integrated approach is applied. This method involves geological studies, field measurements of pore fluid pressure and temperatures, chemistry as well as laboratory investigations of solution properties and solutes content.

This research is part of a joint project between the Frei Universität of Berlin (FU), the Brandenburgische Technische Universität of Cottbus (BTU) and the GeoForschungsZentrum Potsdam (GFZ). Hydrochemical analyses were performed at the FU by Maja Tesmer and interpreted in collaboration with Peter Möller (GFZ) while fluid properties were derived at the BTU, Cottbus, by Christoph Jahnke.

In the next paragraphs, particular attention will be given on the available data of the NEGB system with regard to the aquifer and the fluid model. The state and the processes of fluid migration in the NEGB will be described on the basis of these dataset in order to yield a regional picture of the dominating processes and to derive input data and control parameters for the numerical simulation.

1.2.1 Database and sampling locations

In order to improve the database, the ‘grey’ (unpublished) literature existing at the Geological Surveys of the federal districts of Germany and at commercial companies has been evaluated and organized in a digital database by Christoph Jahnke, BTU. This database contains lithological and petrophysical data, hydrochemical, hydraulic, and geothermal data from about 500 deep boreholes within the study area from Cretaceous to Permian/Carboniferous as well as several thousand datasets from superficial Cainozoic aquifers. The data are mostly from the 1960s to the 1980s. Fig.1-3 (left) illustrates the sampling location of the aquifer parameters. The data provided by Christoph Jahnke include stratigraphic and lithological logs, geophysical/petrophysical logs, data of reservoir tests and analysis of core material which provide input data for the physical parameters of the different stratigraphic units. The sampling location of the data for fluid chemistry and dynamics of saline waters (from Cenozoic to Paleozoic) are shown in Fig.1-3 (right).

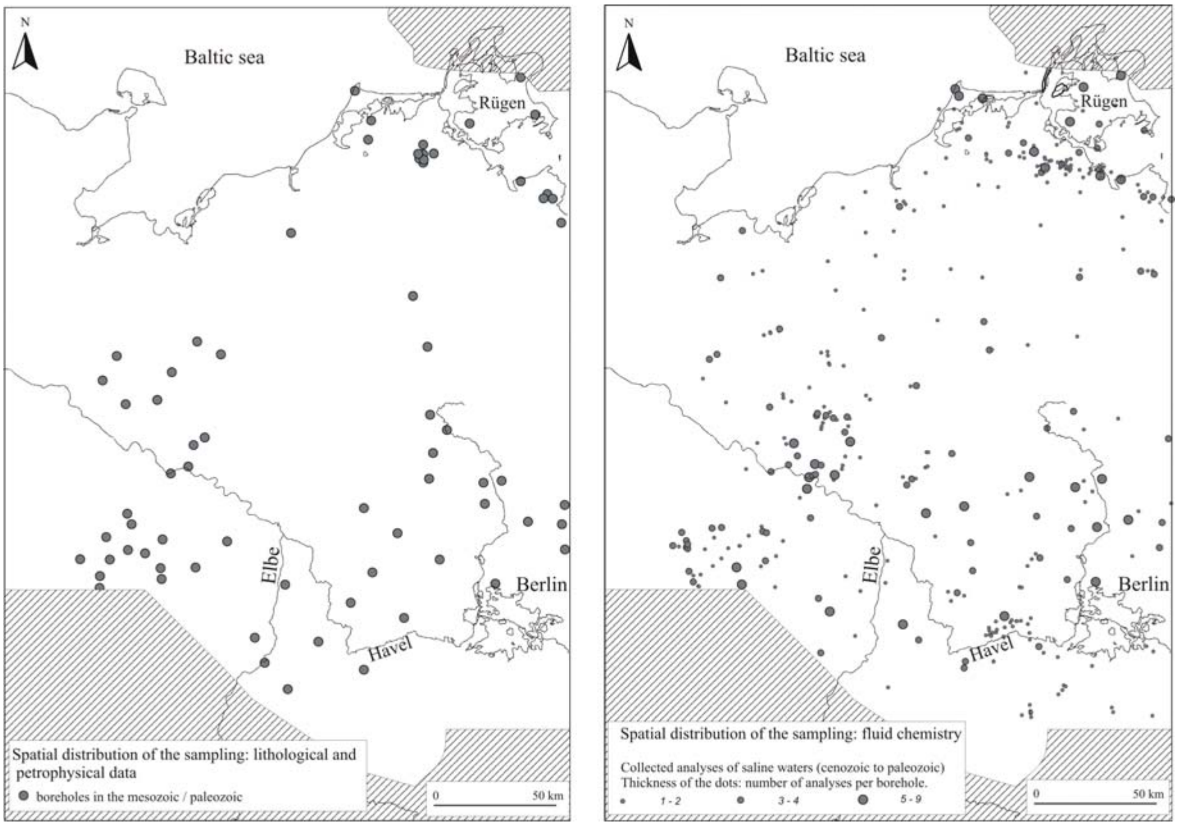

Fig.1-3: Sampling locations for the lithological and petrophysical data (**left**), and for the chemistry and dynamics of deep and saline fluids (**right**). (provided by C. Jahnke, BTU)

These data include chemical analyses of fluids as well as measurements of fluid pressures, hydraulic heads and temperatures which provide indication on the origin and dynamics of salt migration. The available data for fluid chemistry and dynamics are mainly clustered at the centres of the former oil and gas exploration activities and represent a good sampling distribution over the entire study area (in the north: Rügen and Barth-Grimmener structure; in the south-east: Lausatia; in the west: Altmark region).

1.2.2 Aquifer model

The incorporated geological data are derived from a three-dimensional structural model of the NEGB (Scheck 1997; Scheck and Bayer 1999). The area covered by the model is approximately 230 x 330 km in the horizontal extension and 30 km in the vertical direction which consists of 13 layers of the sedimentary fill. Figure 1-4 illustrates the relief of the Top Zechstein Salt derived from the geological input data. The NEGB is affected by intense salt tectonics. Thick salt diapirs pierce more than 4 km of overlying Mesozoic and Cenozoic strata. Salt crests can also be found 500 m below the surface level. Therefore depth and thickness of sedimentation sequences vary strongly within the basin.

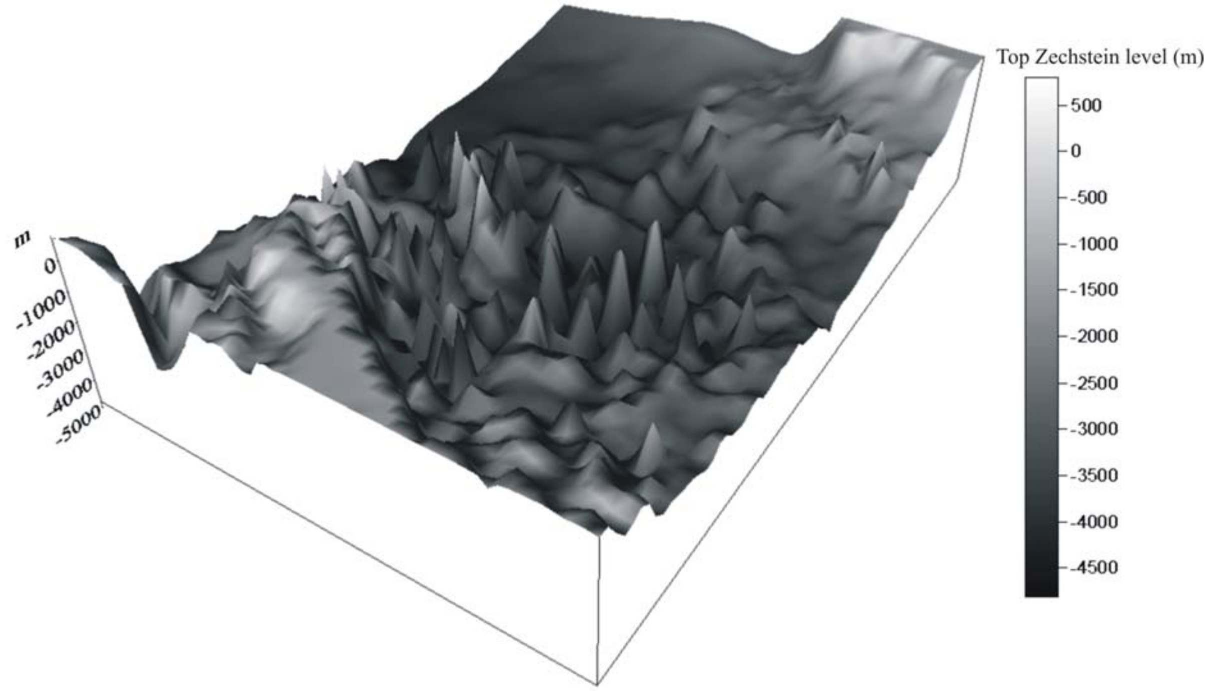

Fig.1-4: Relief of the Top Zechstein derived from the geological input data (Scheck 1997; Scheck and Bayer 1999).

The physical parameters of the sedimentary layer are those given by Scheck (1997, Tab.1). The physical properties considered within each layer are constant. This first rough aquifer model differentiates only the stratigraphic layers of the model without any spatial variation. The development of a detailed aquifer model with spatial variations of porosities, permeabilities, etc., corresponding to the collected petrophysical data is the aim of further research. Furthermore, local faults are not included.

By comparing the hydraulic permeability of the Muschelkalk with those of the younger sediments (Tab.1-1), it turns out that the value is five orders less than the average. Therefore it can be inferred that this stratigraphic formation behaves as a quasi-impervious unit. The Muschelkalk is mainly dominated by fine grained carbonates. Particularly, in the central part of the basin it contains evaporatic layers of salt rock up to some decametres with very low permeabilities. This impervious unit leads to a separation of the Post-Permian strata in two aquifer systems with different hydrochemical and hydrodynamical characteristics (from Lower to Upper Buntsandstein and from Keuper to Cretaceous).

Layer	**Abbreviations**	**Permeability**	**Porosity**	ρ_s	**Heat capacity**	**Heat conductivity**
					Bulk properties	
		[m^2]	**[--]**	**[kg/m^3]**	**[J/(kg*K)]**	**[J/(K*m*s)]**
Cenozoic	Cz	1.e-12	0.23	2670	1180	1.5
Upper Cretaceous	K_1	1.e-13	0.10	2400	1000	1.9
Lower Cretaceous	K_2	1.e-13	0.13	2700	1180	2
Jurassic	J	1.e-13	0.13	2700	1180	2
Upper Triassic	$T_{2\text{-}3}$	1.e-14	0.06	2700	1180	2.3
Middle Triassic	T_2	1.e-18	0.00	2400	1000	1.85
Lower Triassic	T_1	1.e-14	0.04	2670	1180	2
Zechstein (Salt)		1.e-30	~0.0	2160	840	3.5
Elbe Group		1.e-14	0.03	2670	1000	1.84
Mirrow Formation		1.e-14	0.03	2670	1000	2.13
Volcanics		1.e-14	0.03	2670	1000	2.4
Top basement		1.e-30	~0.0	2650	930	2.5
Top mantle		1.e-30	~0.0	2700	1000	2.65

Table.1-1 Physical parameters assigned to the stratigraphic layers.

From the geological model some considerations concerning its influence on regional flow in transporting solute within the NEGB can be inferred. Fig.1-5 (left) illustrates the topography of the top Zechstein Salt which has been derived from the geological input data (Scheck 1997) together with the distribution of saline groundwater (depicted with shaded patterns) as shown in Grube et al. (2000). Grey filled circles locate the position of the observed springs (Schirrmeister 1996). In Fig.1-5 (left), dark patches show the occurrence of salt domes while light grey areas are associated with thin deeper salt pillows. From an analysis of Fig.1-5, no obvious spatial correlation between salt structures and near surface salt occurrences can be inferred. Brine patterns can also be found far away from salt dome crests. This observation already suggests that the regional groundwater flow plays an important role in driving solute. This hypothesis is further supported by comparing the distribution of saline groundwater with the topography of the NEGB as illustrated in Fig.1-5 (right). Although the topography variation is low, it can be seen that the main brine pattern stretches in the lowland along the rivers systems. Nevertheless, some salty plumes can also be observed in regions far from this area suggesting that regional flow, induced by topography, is not the only process transporting solute within the basin.

1.2.3 Fluid model: fluid chemistry and density model

Fluid chemistry

The hydrochemistry of deep saline waters in the Northern German Basin was investigated by Glander and Schirrmeister (1975), Hoth et al. (1997), Hannemann and Schirrmeister (1998), Huenges (2002), Kühn (1997), Lehmann (1974a, 1974b), Löhnert et al. (1986), Müller and Papendieck (1975), Naumann (2000), Neumann (1975), Rockel et al. (1997), Rutter (1988), Thomas (1994), Trettin et al.;(1990, 1997), Voigt;(1972, 1975, 1977). These studies focussed on subjects such as geochemistry, geothermal energy, oil field waters, isotopes, and environmental aspects and thus will not be discussed in detail here. Hannemann and Schirrmeister (1998) concluded that the waters of the springs waters originated mainly in the deeper Pre-Tertiary sub-ground. The steep rising plumes observed in Schleswig-Holstein point to possibly significant temperature effects on the fluid density in addition to any existing forced convection. An overview is given in Grube et al. (2000).

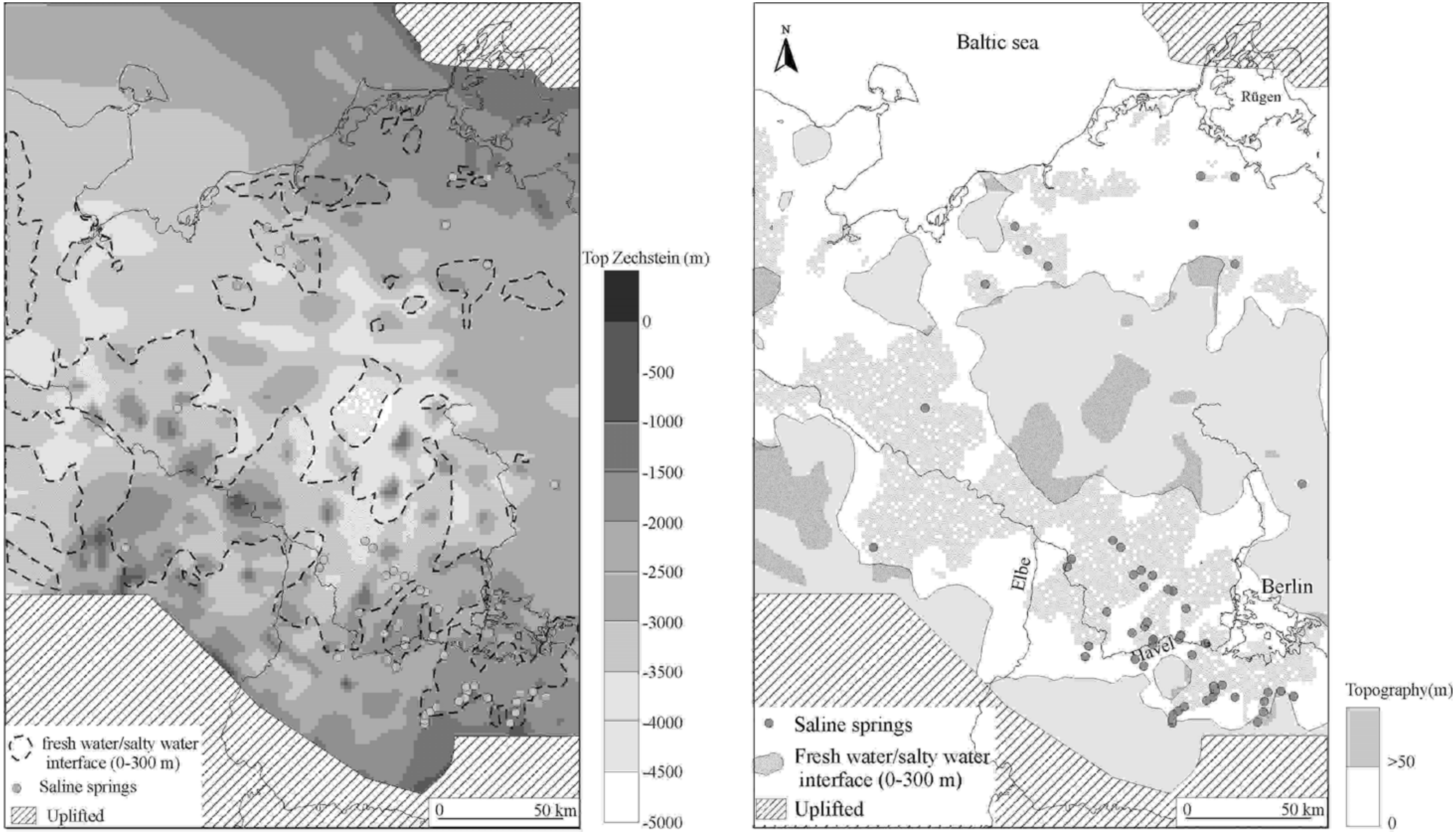

Fig.1-5: **Left:**Top Zechstein depth map (Scheck 1997), location of the observed springs (Schirrmeister 1996) and salty groundwater interface (Grube et al. 2000). **Right**: NEGB topography (Scheck 1997), location of the observed springs (Schirrmeister 1996) and salty groundwater interface (Grube et al. 2000).

The chemical data have been analysed for major and minor ions, ^{1}H/D and ^{16}O/^{18}O by Maja Tesmer (FU). In addition, new investigations on brine chemistry have been performed. At each location, samples for anions and cations, Rare Earth Element and Yttrium (REY), δ^{18}O, δD, and SiO$_2$-geothermometer have been sampled. Where no former analyses for ^{34}S/^{32}S -, ^{13}C/^{12}C- and ^{3}He/^{4}He – isotope ratio and tritium existed, new samples for these isotopes have also been taken. Samples have been stored at 4°C and full water analysis has been generally performed as soon as possible. Sampling and analyses followed the directives of DVWK (1992), DIN (1986). A description of stable isotopes can be found in Meyer et al. Meyer et al. (2000) and for REY in Möller et al. (2003). REY analyses have been normalized by C1-Chondrite.

From the hydrochemistry analysis it emerges that the groundwater salinity increases with depth in the NEGB. Fig.1-6 illustrates the depth salinity trend of groundwater samples in relation to the different stratigraphic units. Salinity is expressed in mg/l of Total Dissolved Solids (TDS).

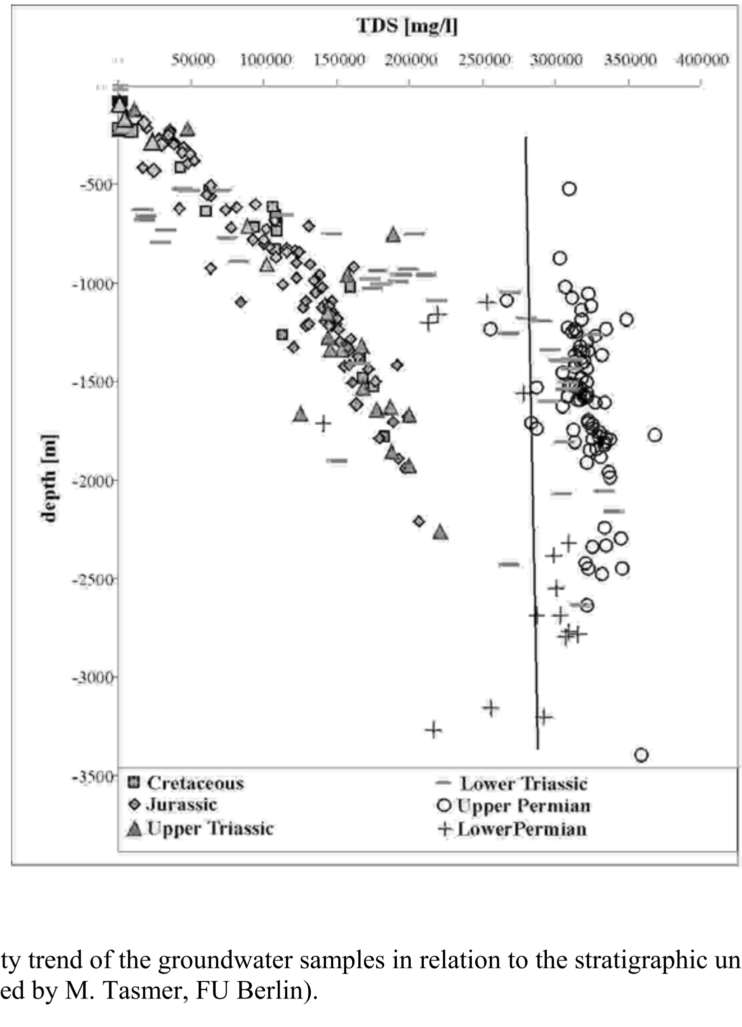

Fig 1-6: Depth-salinity trend of the groundwater samples in relation to the stratigraphic units of the NEGB (provided by M. Tasmer, FU Berlin).

From this figure it can be inferred that a salinity-depth dependency can be assumed for groundwaters belonging to the stratigraphic units from Cretaceous to Upper Triassic (Keuper). On the other hand, the salinity of Permian and Lower Triassic waters are depth independent showing that a saturation level of approximately 345 g/L is reached.

Cluster analyses have been performed by Maja Tesmer (FU, Berlin) to separate hydrochemically different population. Two main hydrochemical groups have been thereby distinguished. A first group consists of nearly pure NaCl waters. Salinity of this type of groundwater predominantly originates in dissolution of halite. This statement is further supported by recent data findings. In the second group, hydrochemical diversity is much higher since cation composition is not restricted to Na^+, but is also affected by Mg^{2+} and Ca^{2+}. On the other hand the overall dominant anion is always Cl^-.

Stable isotope content has been used to get a deeper insight into processes of groundwater salinity while from REY pattern the movement of groundwater between aquifers can be deduced. These chemical data interpretations were carried out by Maja Tesmer (FU) and P. Möller (GFZ). More details can be found in Tesmer et al. submitted). Isotopic contents show that all groundwater samples were built by infiltrating waters, although climatically different recharge conditions were encountered. In general, isotopic contents increase with salinity and depth below -500 m.

For aquifer systems above this level no salinity dependency can be inferred. Therefore mixing processes between waters built under recent or Pleistocene recharge conditions and waters built in warmer periods are supposed to reach this depth driven by topography-induced flow. Interaquifer flow is proven by the REY patterns, especially for shallower aquifer systems. REY patterns additionally prove that even at depth lower than -1500 m interaquifer flow is possible and can be assumed to be ascending.

In summary, chemistry analysis results point toward the main source of salinity from halite dissolution. Salt content increases with depth until it reaches a saturation point estimated around 345 g/l. Isotopic contents indicate that the regional groundwater flow affects the water cycle down to a depth of at least -500 m. REY patterns show the existence of communicating aquifers characterized by upward brine flow.

Fluid density

In geothermal systems temperature and pressure effects on fluid density must be taken into account. Since these influences were neglected in former investigations, fluid density data needed in situ temperature and pressure corrections. The latter have been performed by Christoph Jahnke (BTU).

Fig.1-7 illustrates the density/depth relation in the different pre-Cenozoic aquifers. Approximate density/depth relations were fitted by Christoph Jahnke to the experimental data for the Cretaceous to Keuper, Buntsandstein and Zechstein (Fig.1-7a, b, c respectively). The density values are obtained from laboratory analyses and approximated in-situ densities. In each pictures, the square dots represent the density values obtained from laboratory analysis measured at room temperature. The interpolated average trend is then illustrated by the grey line. The approximated in-situ densities is distinguished by the bold black line. For the determination of the in-situ densities a temperature and pressure correction of the laboratory data was performed. For this purpose an iteration procedure was carried out. Based on the assumption of a simple temperature model and hydrostatic conditions, temperature-corrected densities and pressures were calculated. The temperature model considers only a depth dependency of the temperature (no spatial variations). A thermal gradient of 35 °C/km was assumed for the Mesozoic strata corresponding to geothermal data (Hurtig 1994).

For the Cretaceous to Keuper (Fig.1-7a) the laboratory and in-situ values show a general increase of the fluid density with depth however, with wide scattering. On the other hand, in the Buntsandstein (Fig.1-7b), once NaCl saturation is reached the densities remain nearly constant at about 1220 g/dm^3. At approximately -1.5 km depth the NaCl saturation is reached and at laboratory conditions the density remains close to 1220 g/L. The corrected density/depth temperature relation indicates that the density decreases with increasing depth after saturation has been reached. The inversion of the density/depth trend is due to the thermal expansion of the fluid: at saturation depth, temperature effects are dominating and increase the brine volume which leads to a decrease of its density. Accordingly, the fluid density stratification is unstable and promotes convective flows. Within the Cretaceous to the Keuper this effect may also occur but at depths below 3.500 m. In the Zechstein Salt (Fig.1-7c) the laboratory values indicate that the fluid saturation level is already reached (i.e. the density value is close to 1120 g/L independently of depth). The corrected density/depth temperature relation shows the same inversion trend already observed in the Buntsandstein.

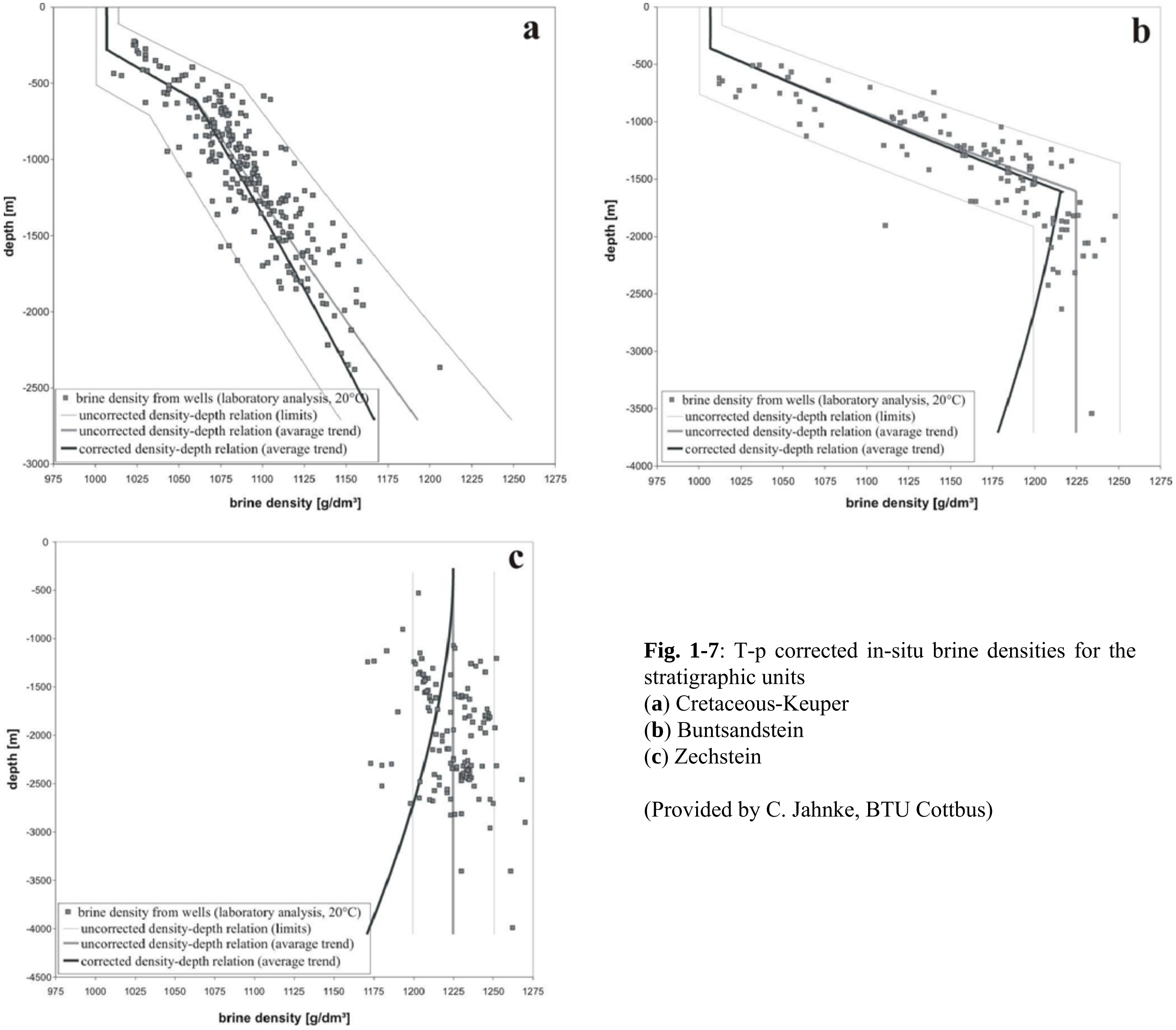

Fig. 1-7: T-p corrected in-situ brine densities for the stratigraphic units
(**a**) Cretaceous-Keuper
(**b**) Buntsandstein
(**c**) Zechstein

(Provided by C. Jahnke, BTU Cottbus)

Fig.1-8 provides an overview about the spatial distribution of the density in some subsurface aquifers. For the Cretaceous to Keuper the density increases from the borders of the basin towards its centre, paralleling depth. The base of Jurassic shows also this typical trend (Fig.1-8a). Spatial deviations exist due to salt diapir occurrence. The Top Buntsandstein, however, shows a very different behaviour (Fig. 1-8b). At lower depth the density increases from the border to the centre due to an increase of salt content. Once NaCl saturation is reached, the density decreases according to the temperature effect. Therefore, the centre of the basin contains fluids with lower density surrounded by a ring of denser waters. This effect becomes stronger with depth and it is more distinctive at the base of the Buntsandstein (Fig.1-8c).

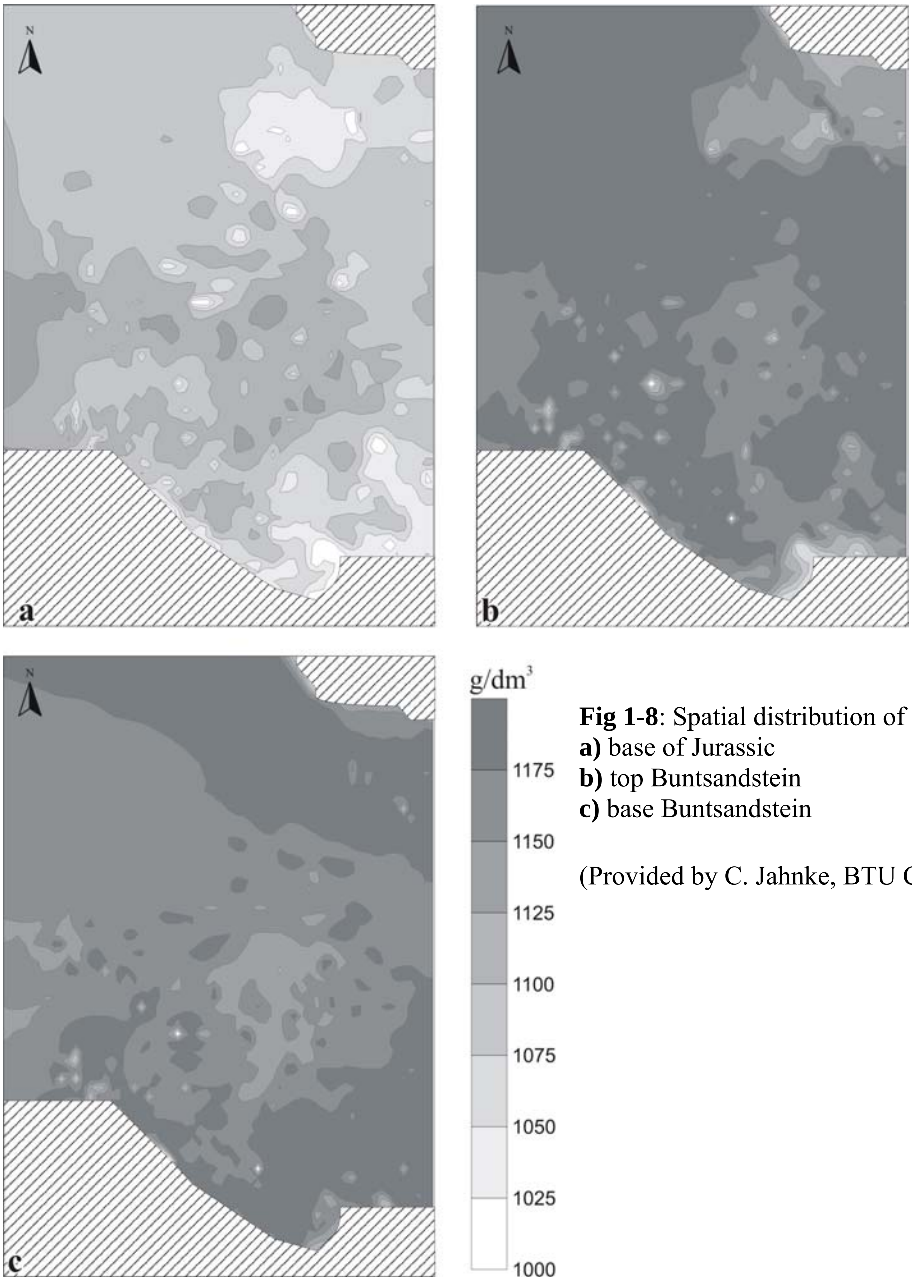

Fig 1-8: Spatial distribution of the density within:
a) base of Jurassic
b) top Buntsandstein
c) base Buntsandstein

(Provided by C. Jahnke, BTU Cottbus)

In summary, the density data point toward a profile sensitive to temperature variations and an unstable condition in the deepest stratigraphic units. Consequently, it can be presumed that thermal buoyant effects are among the major driving forces eventually generating convective flow. Moreover the regional variable density stratification is also unstable and can lead to upward fluid flow depending on the permeabilities of the aquifers.

Fig.1-9 illustrates the pressure gradients within different stratigraphic units of the NEGB. The horizontal intervals depicted in Fig. 1-9 represents the hydrostatic pressure ranges. The pressure gradients above the Zechstein were derived from in situ-densities and correspond well to experimentally obtained data from hydraulic tests (Neumann 1975; Voigt 1975; Rutter 1988). In all stratigraphic units above the Zechstein the pressures are hydrostatic. Therefore the aquifers above the Zechstein can be considered intercommunicating and inter-aquifer flows can occur. Pressures above the hydrostatic level arise only in the Zechstein and in some local zones in the Rotliegend (Voigt 1975).

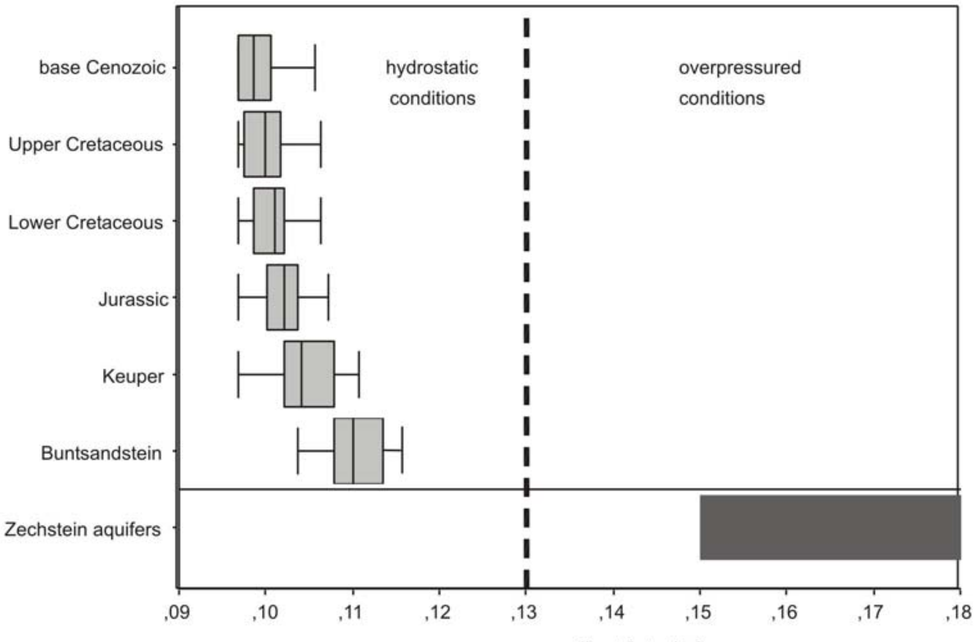

Fig 1-9: Corrected pressure gradients in the different stratigraphic units of the NEGB. (Provided by C. Jahnke, BTU Cottbus)

1.3. Discussion and approaches

The data provide a regional picture of the dominating processes affecting solute transport within the NEGB as well as input parameters for the numerical simulations. The influence of a topography-induced flow regime on salt migration is supported by observations considerations and by isotopic content analysis. These hydrochemical analysis indicate that the regional groundwater flow affects the water cycle down to a depth of at least -500 m. Furthermore the REY patterns highlighted the existence of upward directed inter-aquifer flow even at depth below -1500 m. Therefore intrinsic basin-system mechanisms must exist to exceed the gravity field that would keep dense salt-laden waters in deep seated aquifers. Hydrostatic pressures arise in all stratigraphic units above the Zechstein, suggesting that ascending flows are not due to the existence of any over-pressured aquifers. On the other hand, the fluid density analysis proved that temperature effects lead to a highly unstable density stratification in which denser fluids overly lighter fluids. Consequently thermally induced convective flows are likely favoured. In summary, the data point toward mixed convection.

The data allow to make some preliminary assumptions for the numerical simulations. In the numerical model the brine can be considered pure NaCl solution resulting from halite dissolution. The saturation concentration of the fluid is reached at 345 g/L of dissolved halite which corresponds to a brine density of 1220 g/L. Furthermore, topography-induced flow and fluid density variations described in 1.2.3 must be incorporated.

The thesis will supply insight on the dynamic aspects of geothermal reservoir such as the interaction of the structural setting, the thermal field and fluid-dynamics within the different strata of the basin.

Since this research is centered on the understanding of the system dynamics rather than the development of modelling tools, the strongly coupled non linear equations governing thermohaline convection in porous media will be solved by the use of the commercial Finite Element (FE) program FEFLOW® (Finite Element subsurface FLOW system), WASY GmbH (Diersch 2002).

Thermohaline simulations of different conceptual models of the NEGB shall provide a sufficiently deep understanding of the physics and the numerical modelling of non-linear transport in a given geological system. Moreover, an adequate modelling strategy will be helpful to identify numerical problems and to develop stable numerical solutions.

Finally, using the experience from a stable 2-D model, an effort in building a 3-D model will be made.

This thesis is an attempt to describe in detail the steps taken to tackle the problem.. This applicative work shall present the computational modelling of convective dynamics in the NEGB by undertaking the following steps:

- Integration of the NEGB digital structural model and its related physical parameters by use of FEFLOW®. From this 3-D structural and physical model, a representative 2-D vertical cross-section of the basin will be obtained.
- The transient thermohaline simulations will comprise:
    1) The implementation in FEFLOW of an appropriate equation of state for the density brine that takes in account the effect of pressure, heat and salt.
    2) Stability analysis of the non-linear coupling process by testing different finite element grids.
    3) Testing an alternative set of boundary conditions with the attempt to reproduce observed data.
    4) A successful strategy in developing numerical stable solutions will be tracked down and the computed results will be analysed in order to highlight which factors and geological units allow or prevent convective flow within the basin.
- The 2-D modelling approach will yield fundamental informations concerning the limits and expenses of large scale numerical simulation of density driven fluid-flow with regards to mesh resolution. The knowledge acquired from these 2-D simulations will be used for numerically modelling 3-D thermohaline convection in the NEGB. For this purpose two different FE mesh are applied:
    1) A first rough numerical model scenario will be defined on the whole studied area.
    2) A highly refined grid resolution will be applied on a reduced part of the model.

Finally the results of the simulations will be summarized and discussed.