Temperature fields, petroleum maturation and fluid flow in the vicinity of salt domes

5.5.1 Introduction

Salt domes (diapirs) are common geological features of sedimentary basins. Owing to their physical and structural properties, salt diapirs strongly influence the temperature field of sedimentary basins. This has a great impact on the maturity of organic matter and the timing of hydrocarbon generation. Furthermore, temperature disturbances in the vicinity of salt domes strongly control groundwater transport processes since they provide the coupling between hydraulic and thermally-driven forces.

This chapter consists of three parts. In the first part, the temperature anomalies around salt structures are illustrated. An example based on a salt diapir of the Central European Basin System (CEBS) will elucidate the effects of thermal anomalies on oil maturation. In the second part, an example of fluid flow inside salt structures is given, and in the third part particular focus will be placed on the effects of salt-induced temperature disturbances on groundwater flow processes. Numerical examples of thermally-driven brine flow based on the North East German Basin (NEGB) are subsequently described.

5.5.2 Impact of salt structures on temperature field and oil maturation

5.5.2.1 General Concept

Salt has a thermal conductivity two to four times greater than that of other sedimentary rocks. Values can be as high as 5 to 6 W m⁻¹ K⁻¹ (Cermak and Rybach 1982; Lerche and O’Brien 1987). Therefore, a salt dome buried in strata of much lower thermal conductivity will act as a conduit for heat transport vertically and horizontally. This preferential path for heat conduction causes high-temperature anomalies in the surrounding sediments, as reported in many basins (Bayer et al. 1997; Vosteen et al. 2004). The temperature anomaly is defined as the difference between the temperature observed at a point and the regional trend at that subsurface depth.

The magnitude of the temperature disturbances depends on the size, shape and depth of the salt diapir as described in detail by O’Brien and Lerche (1987, 1988) and Yu et al. (1992). Positive and negative anomalies are found respectively above and beneath salt structures. Figure 5.5.1 shows the contours of the temperature anomaly generated by a single salt dome (O’Brien and Lerche 1987). The largest positive and negative temperature anomalies are to be expected at the top and bottom of the salt dome, while the anomaly goes to zero along a surface which passes through the middle of the dome. The temperature anomaly also extends beyond the edges of the salt dome. Furthermore, there are considerable temperature differences between internal positions in the salt and external positions in the sediments. Sedimentary basins, however, host multiple salt bodies so that their individual thermal effects are mutually interfering and appear as combined temperature pattern (Yu et al. 1992). For example, in the Gulf of Mexico, the anomaly
is as much as 30 °C above salt-bodies and the temperature contrast between internal and external positions is as much as 50 °C (Yu et al. 1992).

So far several studies have been published dealing with temperature anomalies around salt structures. Most of them are theoretical approaches, like Jensen (1990); Petersen and Lerche (1996). Empirical studies in basins containing salt lithologies, for example in the area of the Gulf of Mexico, were published by McBride et al. (1998) and O’Brien and Lerche (1988). Jensen (1983) investigated the temperature field around a salt diapir in Denmark. The published studies in the CEBS are limited to the investigation of the present-day temperature field (Färber 1984) or 2D temperature simulations (Neunzert 1998).

Salt temperature effects are particularly relevant for hydrocarbon thermal maturation (Lerche and Lowrie 1992) since oil accumulations are commonly found in association with salt domes, and oil and gas generation react most sensitively to changes of temperature. Furthermore, thermal disturbances related to salt domes will also have an impact on groundwater transport processes.

With regard to maturation of organic matter, the strong thermal effects of salt structures influence chemical reaction rates. Thermal maturation in sedimentary environments is a kinetically controlled process that can be modelled as a first-order chemical reaction. Therefore, as explained by O’Brien and Lerche (1987) the reaction rates will increase in relation to increased temperature gradients, i.e., on the upper flanks of salt diapirs. On the other hand, on the lower flanks of the salt diapirs, the reaction rates will be lowered. As a result, an enhancement of thermal maturation of any organic matter rich source rock can be expected near the top of the salt. Likewise, negative temperature anomalies will lower or even prevent the maturation of organic matter at the base of the salt diapirs. In general the impact of salt-related thermal disturbances is to enlarge the hydrocarbon window.

Clearly, the timing of salt movement and changes in the shape of salt domes over time are very important in order to simulate the correct thermal and maturity history in the vicinity of a salt plug. For this purpose accurate seismic interpretation and structural balancing are prerequisite. The next section illustrates an example based on the Büsum salt diapir (CEBS).

5.5.2.2 The example of the Büsum salt diapir

One of the prominent salt structures of the CEBS is the salt diapir Büsum (Fig. 5.5.2). There, a 3D numerical modelling study was performed to investigate the influence of
the salt both on the temperature and maturity field of the surrounding sedimentary rocks as well as the temperature and maturity history since the Permian. Calibration of the model was done with measured bottom hole temperatures and vitrinite reflectance data from wells located in the study area. There is a good data base available for this salt diapir because it seals the Mittelplate field which is the largest oil field in Germany.

Study area

The study area is located in the central part of the North German Basin, in the coastal area of the German North Sea (see Fig. 5.5.2). It covers the salt structure Büsum and its surrounding rim synclines. The salt structure Büsum is a NNE-SSW elongated salt diapir with a northern culmination and salt overhangs surrounding it. It has a length of about 16 km and is 7 km wide. The top of the salt diapir rises from about 1200 m below sea level in the south to about 500 m below sea level in the north. It is one of the double salt walls, which are prominent in the central part of the North German Basin, and is made up of Zechstein and Rotliegend salt with a crestal collapse graben structure at the top of the salt dome. In addition to the salt diapir, there is a salt pillow located to the southeast of the study area, within the Keuper strata. It is assumed that this salt pillow was formed by relocated Permian salt.

Located at the western flank of the salt diapir is the biggest German oil field, called Mittelplate, and thus several exploration and production wells have been drilled in this area, the deepest to a depth of about 3000 m, reaching Liassic strata. Figure 5.5.3 shows a cross section through the salt dome and the adjacent rim synclines.

The Jurassic petroleum system comprises the Upper Liassic oil prone source rock (Posidonia Shale), the Middle Jurassic reservoir sandstones and the Middle Jurassic sealing shales. The oil is stratigraphically trapped at the western flank of the salt diapir Büsum (Grassmann et al. 2005).

Salt model

A 3D model including the salt structure Büsum and its surrounding rim synclines was built (see Fig. 5.5.3). The geometry of the model is based on depth structure maps that were made available by the consortium of RWE Dea AG and Wintershall AG, Germany and completed with depth maps from Baldschuhn et al. (2001). Results from an unpublished gravity modelling study gave the present-day shape of the salt diapir Büsum. The evolution of the salt dome over time was adopted from a 2D structural restoration study while lithology data were adopted from well reports. The 3D model covers an area of about 780 km².

As initial thickness of the Permian salt layer a total thickness of 2500 m was assumed, based on Kockel (1995) and Lokhorst et al. (1998). Based on a mass balance approach palaeo thickness maps of the salt layer were constructed for subsequent time steps, starting from the initial thick-
ness to present-day situation. Best results when modelling complex shapes of salt structures are obtained by using a salt piercing tool, that substitutes selected cells of the 3D mesh at a certain time by a defined lithology including the change of petrophysical properties.

Structural balancing for the salt plug Büsum was performed by RWE Dea AG along two seismic lines crossing the salt plug with the software package 2DMove. Furthermore, several depth maps from different horizons are available. The salt plug Büsum is made up of Rotliegend and Zechstein salt. Wells that were drilled in the rim syncline of the salt plug reached their maximum depth in Liassic strata at about 3000 m.

Vitrinite reflectance

The most important parameter to calibrate simulated thermal histories is the measurement of the thermal maturity of organic matter by means of vitrinite reflectance (VRr) in sediments (Senglaub et al. 2006; Littke et al. this volume). For this purpose dark shales and siltstones were selected for the measurements. The samples were mostly taken from the stratigraphic units Tertiary, Early Cretaceous, Dogger and Liassic up to a depth of about 3000 m (as located in Fig. 5.5.2).

Figure 5.5.4. Vitrinite reflectance data for wells Mittelplate 1 and 2 and calculated trend lines using the algorithm of Sweeney and Burnham (1989)
ling studies, but since about 1990, the EASY%Ro algorithm of Sweeney and Burnham (1990) has mainly been used instead of the TTI approach.

Vitrinite reflectance measurements were performed on the wells Mittelplate 1, Mittelplate A9, Mittelplate A13, Dieksand 1 and Dieksand 4. For this purpose, a ZEISS-Photo-microscope III with a 40/0.85 oil immersion objective under normal light at a wave length of 546 nm was used. The aim was to make a minimum of 50 single measurements on each sample, as recommended by Barker and Pawlewicz (1993), to obtain sufficient measurement accuracy. A summary of vitrinite reflectance data on samples from the greater study area is found in Rodon and Littke (2005). For the analysed samples, the mean reflectance (VRr) was determined. Most of the samples which provided useful data are from Jurassic and Early Cretaceous strata, from depths between 1980 m and 2680 m. The Dogger samples reach values of 0.44% VRr up to 0.71% VRr.

Modelling results

Calibration of the models was performed based on an extensive data set on vitrinite reflectance. In figure 5.5.4, this data set is plotted together with calculated vitrinite reflectance-depth trend lines based on the method of Sweeney and Burnham (1990).

The 3D-model allowed calculation of the complex temperature and maturity field in the vicinity of the Büsum structure. The salt chimney effect due to the high thermal conductivity of the salt leads to relatively low temperatures below the salt and high temperatures above. The temperature difference compared to the rim synclines can reach up to 17 °C. With respect to maturity, there is also a difference of up to 0.2% VRr observed, with a “too low” maturity below and a “too high” maturity above the salt diapirs. This difference can have a significant effect on petroleum generation and accumulation. For example, the coal-bearing Carboniferous rocks underlying the Permian salt tend to be highly mature in parts of the CEBS. In this pre-Permian source rock sequence, high maturity was already reached in pre-Tertiary times; therefore no significant late gas generation during the Tertiary and Quaternary was possible (Neunzert 1998) leading to gas accumulation. Only further south in the area of Lower Saxony was pre-Tertiary maturation less pronounced, allowing for significant methane generation from Carboniferous source rocks (Littke et al. 1995). There, large gas fields exist, including the giant Groningen field. In the north, however, where Carboniferous source rocks were buried to much greater depth, this high maturity will only be reduced below thick salt domes due to the chimney effect (Fig. 5.5.5). Accordingly, there may be “sweet spots” for petroleum exploration in such areas, where less mature Carboniferous source rocks still had methane generation potential during the Tertiary. A different situation exists with respect to oil generation from the major source rock, which is the Liassic Posidonia Shale (Grassmann et al. 2005). This rock is generally immature to early mature or – even worse – eroded in this area. Increased thermal maturity in the vicinity of the upper parts of the salt diapir could be a positive factor here, although burial depth has the greatest influence on petroleum generation (Rodon and Littke 2005).

Figure 5.5.5. Cross section through the Büsum diapir and adjacent rim synclines with temperature isolines (left) and vitrinite reflectance isolines (right).
5.5.3 Fluid flow in salt

An essential element of a petroleum system in sedimentary basins is the presence of a seal. Rock salt is known to be the best seal for hydrocarbon accumulations, based on three key properties: First, in-situ permeability and porosity of rock salt are very low, even at a burial depth of merely 70 m (Casas and Lowenstein 1989; Urai, Schléder et al. this volume). Second, the near isotropic stress state provides resistance to hydrofracturing. Thus, especially under conditions of extension tectonics, rock salt will hydrofracture under a higher fluid pressure than shale does (Hildenbrand and Urai 2003), because the minimum principal stress (s3) is higher. Third, plastic deformation of rock salt in nature is ductile and therefore non-dilatant (e.g., Ingram and Urai 1999; Popp et al. 2001). This is reflected by Downey’s (1984) widely accepted ranking of seals: salt → anhydrite → kerogen-rich shale → clay shale → silty shales → carbonate mudstone → chert. On the other hand, under suitable conditions all rocks can lose their sealing capacity. However, the geological conditions for loss of seal capacity of rock salt are not well known.

As a first step, we should differentiate between fluid flow in rock salt (halite) sensu strictu, and in evaporite sequences. Many salt basins are characterised by the occurrence of carbonate rocks within such evaporitic sequences. In the CEBS these carbonates can act as reservoir rocks for oil and gas, proving that active fluid flow has taken place. In eastern Germany, oil reservoirs are present in Zechstein carbonates. Lateral migration over distances of tens of kilometres has probably charged these reservoirs (Fig. 5.5.6; Hindenberg 1999). This self-charging system exists due to the fact that the carbonates formed the marginal facies of the Zechstein basin. At the same time, in more basinal settings, marls and fine grained carbonates were deposited with higher organic carbon content, possessing a source rock potential. Thus intraformational flow within the carbonates towards the most porous and permeable facies filled the reservoirs which were sealed by rock salt.

Further towards the west, the same carbonates act as gas reservoirs, but also as gas source rocks. Whereas the bulk of the methane gas in this area is derived from Late Carboniferous coal-bearing rocks (Littke et al. 1995),

![Figure 5.5.6.](image-url)
a minor contribution has to be attributed to a carbonate source rock. As these gas pools with “carbonate” signature mainly occur in Rotliegend reservoirs juxtaposed to the Zechstein sequence, it is probable that migration of gas out of the carbonates into the reservoirs has occurred (Littke et al. 1996). In the Lower Saxony Basin constituting the southern part of the CEBS, carbonate stringers are partly in contact with the underlying older strata and not underlain by salt. Some of these carbonates act as gas reservoirs, having vastly different contents of methane and carbon dioxide. In this case, the structural setting seems to be decisive for the quality of the gas filling. In particular, early filling by methane gas from underlying Carboniferous source rocks followed by decoupling from later inflow of carbon dioxide seems to be a prerequisite for the existence of high quality gases (Petmecky 1998; Petmecky et al. 1999; Krooss et al. this volume).

Observations above clearly demonstrate that there is fluid flow taking place into evaporites, out of evaporites and inside evaporites. Furthermore, simple mass balances on total gas generation in the thick Late Carboniferous source rock sequence of the southwestern CEBS prove that much more gas was generated post-Zechstein than is presently trapped (Littke et al. 1995). Accordingly, this gas must have migrated out of the Palaeozoic sequence through the Zechstein evaporites towards the surface.

Nollet et al. (2005) studied vein systems in the Buntsandstein of the CEBS. Based on microstructural and geochemical arguments they proposed a regional high pressure cell during burial of this sequence, with the origin of the fluids in the Zechstein, which must have migrated through the rock salt sequence into the Bunter.

Figure 5.5.7.
Macroscopic (left) and microscopic (right) appearance of solid bitumen in rock salt (Ara salt, Oman; see Schoenherr et al. 2007a,b for details)
These results imply that large scale fluid migration through the evaporitic sequence can be quite common. In-situ permeability of undisturbed rock salt is $\sim 10^{-21}$ $m^2$ (Bredehoeft 1988; Peach and Spiers 1996; Popp et al. 2001). This low permeability allows rock salt to seal large hydrocarbon columns and fluid pressure cells over geological time. Two processes are known to increase permeability. The first is microcracking and associated dilation (Peach and Spiers 1996; Popp et al. 2001), and the second is the formation of topologically connected brine-filled pores and triple-junction tubes in halite grain aggregates at a pressure and temperature corresponding to depths $> 3$ km (Lewis and Holness 1996). In the triaxial deformation experiments of Lux (2005), rock salt became permeable by the formation of grain boundary cracks at low rates of fluid-pressure increase. If the fluid-pressure ($P_f$) is increased rapidly to a sufficiently high excess pressure ($P_f > \sigma$), rock salt leaks by hydrofracturing. Peach and Spiers (1996) proposed that this process could also occur under low effective stress during natural deformation of rock salt at great depth and high pore-fluid pressures. More theoretical background on permeability and microfractures in rock salt is discussed in Schoenherr et al. (2007a) and Urai, Schléder et al. (this volume).

One of the best known examples of oil flow in rock salt is found in the Infra-Cambrian Ara Group of South Oman (Schoenherr et al. 2007b). The Ara Group consists of marine platform sediments, representing at least six third-order cycles of carbonate-evaporite sedimentation, of up to 4 km thickness (Mates and Conway Morris 1990). Each cycle is characterised by sedimentation of up to 1000 m Ara Salt at very shallow water depths, followed by the deposition of 20 to 250 m thick isolated carbonate platforms (the so-called “stringers”) during transgressive periods.

Most of the carbonate stringers contain fluids at very high overpressures. The carbonate stringers have undergone intense diagenetic modifications with locally extensive cementation by halite and solid bitumen (Schoenherr et al. 2007a). They have been interpreted to be a self-charging system with first oil charge from mature Type I/II source rocks (Peters et al. 2003) during the early Cambrian to Ordovician at maximum burial temperatures after deposition of the overlying Haima Supergroup (Visser 1991; Terken et al. 2001). In addition, geochemical studies suggest external (pre-Ara) oil and gas charge (Al-Siyabi 2005).

Presence of solid bitumen as a relic of former oil is evident from macroscopic observations not only in the carbonates (where it may be expected), but also in the rock salt (Fig. 5.5.7, left; Schoenherr et al. 2007a). Microscopy revealed that solid bitumen is both present on grain boundaries and in microcracks (Fig. 5.5.7, right). The black rock salt cores clearly indicate that distinct parts of the Ara Salt lost sealing capacity for oil. Oil initially leaked into the salt when oil pressure in the reservoir exceeded the near-lithostatic fluid pressures of the Ara Salt by a few tenths of a MPa to overcome the capillary entry pressure, followed by diffuse dilation and marked increase in permeability, in agreement with laboratory-calibrated dilation criteria of rock salt. Oil could flow into the salt as long as the oil pressure remained larger than the minimum principal stress in the rock salt. A detailed explanation is given in Schoenherr et al. (2007a,b). The conditions inferred from this study represent the ultimate sealing potential of rock salt in the deep subsurface, and can be applied to rock salt seals in any tectonic setting. Another study of fluid flow in salt is presented in by Schléder and Urai (2005), see also Urai, Schléder et al. (this volume).

In summary, lithostatic fluid pressures increase the permeability of rock salt by many orders of magnitude, allowing flow of water and hydrocarbons until the fluid pressures decrease. There is increasing evidence that this has occurred in many salt-bearing basins, providing an explanation for many observations, and an indication for palaeo-overpressures.

5.5.4 Impact of salt structures on groundwater transport processes within sedimentary basins

In this paragraph, the effects of salt-induced temperature disturbances on groundwater transport are described. For this purpose, a brief overview of the main driving forces of groundwater flow in sedimentary basins is given. Then numerical examples based on the North East German Basin (NEGB) will serve to illustrate the principle impact of salt domes on thermally-driven brine flow.

5.5.4.1 Brief description of driving forces in large-scale groundwater flow systems

Sedimentary basins are subjected to several forces known to cause large-scale groundwater migration, each characterised by a typical flow rate as reviewed by Bjørlykke et al. (1988); Garven (1995); Person et al. (1996) and Ingebritsen and Sanford (1998).

Topography-driven flow (Fig. 5.5.8A) is the dominant regional-scale groundwater flow in sedimentary basins both in the shallow and deep sub-surface (Freeze and
Witherspoon 1967). This regional flow occurs when differences in the hydrostatic head drive fluid from high-elevation recharge areas to low-elevation discharge areas. Flow lines and rates depend on several factors as the geometry of the aquifers and their physical properties (e.g., hydraulic permeability). Typical maximum flow rates range from 1 to 10 m year⁻¹.

In sedimentary basins, the presence of chemical compounds and/or the geothermal field induce fluid-density variations which in turn drive groundwater flow. Fluid motion caused by density difference due to temperature variations is called free convection (Fig. 5.5.8B) while gravitational convection is the term used when the convective currents are induced by variations in solute concentration.

Ongoing geological processes such as sediment compaction, tectonic compression (Fig. 5.5.8C), hydrocarbon generation or degassing of magma can induce significant fluid flow. These processes are referred to as geological forcing (Neuzil 1995) and their flow rates span a large range of velocities. For example, compactionally driven pore-water flow rates are usually very slow, in the order of $10^{-6}$ to $10^{-3}$ m year⁻¹, while tectonic compression can induce flow rates of 0.5 m year⁻¹ (Garven 1995).

These processes are coupled!

An important feature of deep groundwater flow within sedimentary basins is that mechanical, hydrological, thermal, and chemical mass transfer processes are fully coupled.
Transport processes take place over large temporal scales during which basin deformations are often substantial. Therefore, there is a mechanical coupling between the driving forces and the structural evolution of the basin. Furthermore, increases in sub-surface fluid pressures induce rock dilation and porosity increase. In contrast, mineral precipitation reduces rock porosity, decreasing groundwater flow rates (Garven 1995). Over the large spatial scales encountered in geothermal basins, temperature and solute concentration strongly vary. These variations modify the physical properties of both fluid (density, viscosity) and rock units (hydraulic conductivity, porosity) leading to new dynamic effects of the system.

The archetypal example for sedimentary basins is the coupling of heat and dissolved halite which have different rates of diffusion (heat diffuses faster than salt): the flow is then called thermohaline convection (Nield and Bejan 1999). Since in geothermal basins the temperature gradients increase with depth, heat acts as a destabilising potential. Two major scenarios for thermohaline convection to occur can be distinguished. (i) When salt concentration increases with depth (salinity is stabilising), the deeper brines are heated from below and therefore less dense: an upward flow is triggered leading to the formation of convective cells (Fig. 5.5.9 top). As the flow progresses, the brines will cool off quickly while losing little salt diminishing the upward buoyancy force. Eventually, brine will start sinking. (ii) Another possible scenario is when salinity gradients also act as destabilising factors. That is the case when brine forms in shallow areas of the basin (e.g., from shallow salt structures). The denser fluid will therefore sink into the deeper and hotter part of the basin. At the same time, lighter and hotter fluids will move upward.

Figure 5.5.9. Top thermally induced brine plumes developing from a deep salt sheet. Bottom brine lenses induced by an instable density stratification and thermohaline convection. The bold vectors indicate the direction of the cellular motion, the dashed lines are the isotherms in °C.
Box 5.5.1 Mathematical formulation of the thermohaline flow problem

The governing equations of thermohaline convection in a saturated porous media are derived from the conservation principles of linear momentum, mass and energy (e.g., Kolditz et al. 1998; Nield and Bejan 1999). They are briefly reported here by the following set of differential equations:

\[ S_0 \frac{\partial \rho}{\partial t} + \text{div}(\mathbf{q}) = Q_{\text{Boussinesq}} \quad (5.5.1) \]

\[ \mathbf{q} = -K \left( \text{grad}(\mathbf{p}) + \frac{\rho_f - \rho_s}{\rho_0} \right) \quad (5.5.2) \]

\[ \frac{\partial \phi}{\partial t} + \text{div}(\text{qC}) - \text{div}(\text{Dgrad}(\mathbf{C})) = Q_c \quad (5.5.3) \]

\[ \frac{\partial}{\partial t} \left( \beta_f \phi \mathbf{c}_f + (1-\phi) \rho_f \mathbf{c}_s \mathbf{T} \right) + \text{div}(\rho_f \mathbf{c}_f \mathbf{T}_0) = \text{div} \left( \lambda \text{grad}(\mathbf{T}) \right) = Q^f \quad (5.5.4) \]

Equation 5.5.1 is the equation of fluid mass conservation. \( S_0 \) is the medium storativity which physically represents the volume of water released from (or added to) storage in the aquifer per unit volume of aquifer and per unit decline (or rise) of head \( \phi \). \( Q_{\text{Boussinesq}} \) is the Boussinesq term which incorporates first order derivatives of mass-dependent and temperature-dependent compression effects. \( \mathbf{q} \) is the Darcy (or volumetric flux density velocity) defining the specific discharge of the fluid. Darcy’s law is expressed by equation 5.5.2 where \( K \) is the hydraulic conductivity tensor, equation 5.5.3 is the equation of solute mass conservation where \( \phi \) is the porosity of the porous medium, \( C \) is the mass concentration, \( D \) is the tensor of hydrodynamic dispersion and \( Q_c \) is a mass supply. Equation 5.5.4 is the energy balance equation of the fluid and porous media. \( T \) is the temperature, \( \lambda \) is the tensor of hydrodynamic thermodispersion.

Constitutive and phenomenological relations of the different physical parameters involved in the equations are needed to close this coupled system. Here the hydraulic conductivity relation and the equation of state (EOS) for the fluid density are given:

\[ K = \frac{k \rho'_0 g}{\mu_f (C,T)} \quad (5.5.5) \]

\[ \rho'_0 \left( 1 - \frac{\beta_f (T_0, p)(T - T_0) + \gamma (T, p)(p - p_0) + \frac{\alpha}{\Delta C_s - C_0} (C - C_0)}{\rho'_0} \right) \quad (5.5.6) \]

The hydraulic conductivity tensor \( K \) is related to the reference fluid density \( \rho'_0 \), \( g \) is the gravitational acceleration, \( k \) is the tensor of permeability, \( \mu_f (C,T) \) takes into account the fluid viscosity effects due to temperature and concentration variations. The EOS for the fluid density (Eq. 5.5.6) is related to the reference temperature \( T_0 \), pressure \( p_0 \) and concentration \( C_0 \).

\( \beta_f (T, p) \) is the fluid density ratio, \( \rho'_0 \) being the fluid density at saturation. \( \beta_f (T, p) \) is the coefficient of thermal expansion and \( \gamma (T, p) \) is the coefficient of compressibility.

The flow and transport equations (Eq. 5.5.2, 5.5.3, 5.5.4) for thermohaline convection are non-linear and strongly coupled since temperature and salinity control the fluid density \( \rho' \) and dynamic viscosity \( \mu_f (C,T) \). The variation of fluid density is essential for the modelling of thermohaline convection because of its primary importance for calculating the correct buoyant force included in the equation of motion (i.e., generalised Darcy’s law Eq. 5.5.2). Fitted polynomial expressions are commonly used for temperate, pressure and salinity dependences of the fluid density (Sorey 1976).

* Stability criteria

A dimensional analysis of the governing balance equations (Eq. 5.5.1 to 5.5.4) allows the definition of several adimensional numbers (Nield and Bejan 1999). The key dimensionless number is the Rayleigh number (Ra), which is the ratio between buoyancy-driven forces and resisting forces caused by diffusion and dispersion:

\[ \text{Thermal Rayleigh number } Ra_T = \frac{K \beta_f A_T d}{\Lambda} \quad (5.5.7) \]

\[ \text{Solutal Rayleigh number } Ra_s = \frac{\alpha}{C_{sat} - C_0} \frac{K \Delta C_d}{\varepsilon D_d} \quad (5.5.8) \]
owing to the thermally induced buoyant forces. Consequently, brine lenses and convection cells form (Fig. 5.5.9 bottom).

Thermohaline convection can develop cells at flow rates approaching 1 m yr⁻¹ (Evans and Nunn 1989; Garven 1995) which are strong enough to control temperature and concentration fields. On the other hand, vigorous topographically-driven groundwater flow can overwhelm free convection and modify the thermal structure of the basin (forced convection). Precisely, it causes cooling in recharge areas and increase heat flow in discharge areas. Temperature differences up to 50 °C can be expected between recharge and discharge areas (Ingebritsen and Sanford 1998). In some cases, thermally-induced convection and topography-driven flow coexist (Raffensperger and Garven 1995a; Thornton and Wilson 2007) leading to a mixed convection regime.

The onset of thermohaline convection can be derived numerically. The mathematical formulation and the stability criteria for the thermohaline problem are given in Box 1. A key number which controls the flow dynamics is the Rayleigh number. If the Rayleigh number is large enough, then cellular motion can develop. As a result, a multitude of stability analyses based on laboratory experiments were carried out on saturated porous media with vertical gradients of temperature and salinity in order to determine the conditions for convection.
to determine the critical Rayleigh number for the onset of thermohaline convection (Horton and Rogers 1945; Lapwood 1948; Elder 1967; Trevisan and Bejan 1987; Kubitschek and Weidman 2003).

Comment on the drawbacks of adimensional analysis for real basin systems:

While Rayleigh theory can be successfully used for the study of convective flow in homogenous systems, its applicability for transport processes within real sedimentary systems is seriously questioned (Raffensperger and Garven 1995a; Simmons et al. 2001). This criterion assumes that a steady-state flow takes place in a homogeneous system under steady state conditions. A Rayleigh number may be derived for heterogeneous systems provided that the properties vary within only one order of magnitude (Nield 1994). In real-site applications, this is often not the case: the physical parameters of the basin are subject to large heterogeneities. Furthermore, stability analysis based on dimensionless numbers involves the definition of a characteristic length-scale of the porous media (d Box 5.5.1 Fig. 1) through which temperature and solute gradients are supposed to vary linearly. These conditions are not satisfied in any transport processes occurring within real basin systems. Usually, concentration and temperature gradients are non-linear due to salt structure disturbances. The thicknesses of the stratigraphic units of sedimentary basins can vary from a few meters to several kilometers because of the strong salt tectonics. Therefore, the definition of a representative length scale is rather problematic. From these considerations, it follows that the Rayleigh criteria are not appropriate (and perhaps even impossible) for analysing coupled transport processes within real system.

Salt diapirs: a unique geological environment for thermohaline convection

The relative importance of the above mentioned coupled driving forces on fluid flow varies depending on the tectonic and lithologic conditions. It is proven that thermally-induced flow can lead to transport of dissolved compounds over large spatial scales and in significantly shorter times compared with diffusion alone (Hanor 1987; Diersch and Kolditz 2002). Furthermore, it has been shown that thermally-induced flow is a major factor controlling deposition of minerals in basins and, therefore, affecting basins diagenesis. For instance, numerical investigations of coupled transport processes showed that free convection is responsible for ore deposits in the Mc Arthur Basin, Australia (e.g., Garven et al. 2001; Yang et al. 2004a,b) and in the Athabasca Basin, Canada (Raffensperger and Garven 1995a,b). Clearly, any effect which causes a significant variation in temperature gradient will play a fundamental role in determining the groundwater regime. Therefore, owing to their physical properties, salt diapirs provide a unique geological environment for thermohaline convection to occur. In recent decades, the perturbation of the geothermal field associated with salt diapirism has been studied for thermally-induced fluid convection (e.g., Fogg et al. 1983; Hanor 1987; Ranganathan and Hanor 1988; Evans and Nunn 1989; Evans et al. 1991; Thornton and Wilson 2007). There are a multitude of environmental circumstances where thermohaline convection can arise, includ-
ing transport of pollutants released from waste disposal in salt rock formation (Evans and Nunn 1989), or salt layers embedded in aquifers (Sarkar et al. 1995) can be mentioned. The Gulf Coast region of the United States is one of many examples and was one of the first case studies of thermohaline convection in salt-dome environments.

5.5.4.2 Example: Gulf Coast region of the United States

The salt domes of the Gulf Coast have been thoroughly explored in the search for oil and gas (Mace et al. 2006). Hydrochemical investigations showed that fluids around several salt domes have anomalous salinities owing to the local dissolution of halite from the salt flanks (Workman and Hanor 1985; Bennet and Hanor 1987; Enos and Kyle 2002). Groundwater that is in contact with the salt dome reaches concentrations up to saturation level (i.e., 345 g/L). Plumes of dense saline water are gravitationally unstable and have the potential to sink. Furthermore, hydrochemical patterns indicate that warm fluids from deep formations discharge into shallower units. The coupling of these downward and upward migrating fluids is likely to form convective flow systems of 1 km diameter. A comprehensive review of fluid-rock interaction in salt-dome environments for this area is given by Posey and Kyle (1988).

Numerical models were built in order to investigate the feasibility of these flows. According to the Ranganathan and Hanor models (1988) salinity-driven convection cells (Workman and Hanor 1985; Bennet and Hanor 1987; Enos and Kyle 2002). Groundwater that is in contact with the salt dome reaches concentrations up to saturation level (i.e., 345 g/L). Plumes of dense saline water are gravitationally unstable and have the potential to sink. Furthermore, hydrochemical patterns indicate that warm fluids from deep formations discharge into shallower units. The coupling of these downward and upward migrating fluids is likely to form convective flow systems of 1 km diameter. A comprehensive review of fluid-rock interaction in salt-dome environments for this area is given by Posey and Kyle (1988).

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achieve maximum flow velocities of 0.01 to 1 m yr\(^{-1}\). Further modelling showed that the temperature disturbances caused by the presence of a salt structure can set up buoyancy forces which have the potential to drive large-scale brine convection (Evans and Nunn 1989; Evans et al. 1991). In their calculation, two distinct kilometre-scale convective cells develop: one cell near the top of the dome with upward flow at the salt edge, and another extending to the bottom of the system with downward flow (Fig. 5.5.10 top). A salt plume extends away from the salt dome as a result of upward flow (Fig. 5.5.10 bottom).

In summary, the disturbed thermal regime around the dome generates an unstable fluid-density stratification which induces upward brine movement along salt flanks. Eventually, warm fluids discharge into the shallower units. However, these models were based on a single salt dome surrounded by homogenous sediments while in sedimentary basins different salt bodies are in close juxtaposition and cut through heterogeneous units. More detailed models with regard to the basin lithology and internal structures are needed in order to understand the geological conditions in which thermally-induced convective flow occurs.

5.5.4.3 Numerical example of thermally-induced flow in relation to salt dome environment (including chemical observations): the N-E German Basin

An interesting example illustrating thermally-driven processes in a sedimentary basin hosting many salt structures is provided by the North-East German Basin (NEGB) as part of the Central European Basin System (CEBS) as described in detail by Magri (2005); Magri et al. (2005a,b, 2007).

**Salty-water evidences in the NEGB**

Extensive evidence for rising saline waters has been gathered in different regions of this basin (Fig. 5.5.11). 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 is occurring in the south-eastern part of the NEGB. Precisely, the majority of the saline springs are observed in the neighbourhood of the Elbe and Havel rivers and to the south of Berlin. Only a few are encountered away from these locations.

Additional evidence of salty groundwater 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. 5.5.11). The photo was taken in 2004 during a field trip to 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.

Although this phenomenon has been observed for decades (Heck 1931; Johannsen 1954; Schirrmeister 1996; Hannemann and Schirrmeister 1998; Grube et al. 1996, 2000), an unsolved feature of these saline springs is their...
temporal and spatial instability. Furthermore, the observed brines at the surface are a few degrees hotter than the average fluid temperature in the soil.

Figure 5.5.12 (left) illustrates the occurrence of shallow salt domes (dark patches) and thin deeper salt pillows (light grey areas) together with the salty groundwater distribution. It can be seen that no obvious spatial correlation between salt structures and near surface salt occurrences exists. Brine patterns can also be found far away from salt dome crests. Most of the salty groundwater stretches are in the lowland along the rivers system (Fig. 5.5.12, right). It can be inferred from this observation that the regional flow induced by topography variation plays an important role in driving solutes. Nevertheless, some salty plumes can also be observed in regions far from this area indicating that regional groundwater flow is not the only process transporting solute within the basin. Furthermore, the topography variation is not great enough to lift deep-seated waters up to the surface.

Hydrochemical patterns in groundwater provide information about possible salinity sources and flow direction. The hydrochemistry of deep saline waters in the Northern German Basin was investigated amongst many others by Lehmann (1974a, b); Voigt (1977); Hannemann and Schirrmeister (1998); Tesmer et al. (2007); Möller et al. (2007b).

The main source of salinity is halite dissolution from the salt domes. Salt content increases with depth until it reaches a saturation point estimated around 345 g/L. The influence of a topography-induced flow regime on salt migration is supported by isotopic analysis which indicate that the regional groundwater flow affects the water cycle down to a depth of at least -500 m (Tesmer et al. 2007). On the other hand, the Rare Earth elements and Yttrium (REY) patterns highlight the existence of upward directed inter-aquifer flow even at a depth below -1500 m (Tesmer et al. 2007; Möller et al. 2007b). Therefore, intrinsic basin-system mechanisms must exist to overcome the gravity field that would keep dense salt-laden waters in deep seated aquifers. Hydrostatic pressures rise in all stratigraphic units above the Zechstein, suggesting that ascending flows are not due to the existence of any over-pressured aquifers. A possible cause could be thermally-induced flow as indicated by fluid density studies.

Fluid density analyses show that from the point of saturation the density decreases with increasing depth. The inversion of the density/depth trend is due to the thermal expansion of the fluid. Precisely, at the saturation depth, temperature effects are dominating and increase the brine volume which leads to a decrease of its density. Within the Cretaceous Keuper interval this effect occurs at depths below 3500 m. Accordingly, the fluid density stratification is unstable and promotes thermally induced convective flows. At this state the question arises, how do salt-induced temperature disturbances drive brine flow?

The numerical simulations presented in the next paragraph will highlight the role these temperature disturbances play in controlling upward solute transport.

The numerical model

Large scale simulation of coupled fluid flow, mass and heat transport based on a real geothermal system requires a proper aquifer and fluid model. The aquifer model should include the structural characteristics of the aquifers as well as the physical parameters such as porosities, hydraulic permeabilities, heat conductivity and heat capacity. The fluid model should take into account the chemical and physical fluid characteristics and their spatial distribution, water salinity, chemical components and fluid density.
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 across and 5 km in depth, consisting of 9 layers of sedimentary fill, including the basement. Figure 5.5.13 illustrates the geological structures of the cross-section used for the numerical simulations. 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 sediment sequences vary greatly within the basin. 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. More details concerning the physical parameters of the sedimentary layers can be found in Magri et al. (2005a). Local faults are not included.

Fluid model

The hydrochemical investigations allow us to make some preliminary assumptions for the fluid model. The brine can be considered pure NaCl solution resulting from halite dissolution. For the brines within the Mesozoic strata this assumption provides a sufficient approximation. 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. In geothermal systems, the influence of pressure, temperature and concentration on the fluid density cannot be neglected.

Two polynomial expressions which accurately represent the coefficient of thermal expansion $\beta(T,p)$ and compressibility $\gamma(T,p)$ for the fluid density (Eq. 5.5.6, Box 5.5.1) have been derived and coded as an extension to the simulation program. A detailed description of these polynomial functions and the implemented code is reported in Magri et al. (2005a).

Modelling approach

The strongly coupled non-linear equations governing thermohaline convection in porous media (Box 5.5.1) are solved by the use of the commercial Finite Element (FE) program FEFLOW® (Finite Element subsurface FLOW system), WASY GmbH.

The resolution of the finite element grid is variable and allows modelling of variations in fluid-density. More details, also on boundary conditions, can be found in Magri et al. (2005a).

Role of salt-induced temperature disturbances on groundwater transport processes: simulation results

Temperature disturbances on brine flow: free thermohaline convection

Figure 5.5.14(AB) shows the calculated transient temperature and brine distribution. The principle result is that
a disturbed profile develops throughout the sediment fill above the Zechstein unit. The oscillatory pattern is characteristic of a multicellular convective regime. The waves are non-periodic and their amplitudes decrease with depth. In the western part of the basin, the temperature isopleths are nearly flat presenting only one anomaly near the salt dome. In the eastern part of the basin, a long way from the salt diapir, the temperature distribution is less disturbed. Below the Zechstein unit the temperature profile is conductive everywhere, showing the well-known thermal anomalies within the salt diapirs (i.e., concave temperature isopleths).

Owing to the strong coupling between heat and mass transfer in thermohaline convection, the saline and thermal plumes developed together spreading over the same areas within the sediment fill (compare Fig. 5.5.14A and B). Above the Muschelkalk, brine plumes develop rapidly and penetrate the overburden (Fig. 5.5.14A). Brine fingers form and extend vertically over 3 km throughout the sediments.

Salty waters with more than 1 g/L of dissolved halite spread over the surface driven by the disturbed geothermal field. At the western part of the basin, the finger regime disappears. The concentration isopleths are flat and the salt content increases almost linearly with depth. The layered brine stratification is probably a boundary effect. Since the lateral boundaries of the model are closed to fluid flow, mass and heat transfer, the dissolved halite cannot diffuse away in the western direction. Moreover, salt diffusion in the eastern direction is also prevented due to the presence of shallow salt diapirs. Therefore, as time progresses, the sediments are filled with halite. The finger regime evolves into a layered system in which concentration increases with depth. At the eastern ending of the
profile, brine plumes do not develop since at that location the temperature gradient is not disturbed.

On the other hand, temperature disturbances play a dominant role on brine migration especially in the neighbourhood of salt diapirs. A zoom of the calculated pore velocity and temperature fields in a salt dome environment is shown in figure 5.5.15A. Downward forces resulting from the gravitational field control groundwater flow along salt diapir flanks. The salt-laden water sinks at approximately 1.5 cm yr⁻¹ (Fig. 5.5.15A). By contrast, an upward flow paralleling this descending flow occurs in the overlying unit at approximately 1 cm yr⁻¹. This phenomenon can be explained by the temperature distribution (Fig. 5.5.15B). Because of the thermal conductivity contrast between salt and overlying sediments the isotherms are convex near the edge of the salt diapir. The increased temperature gradient causes a decrease in fluid density near the salt dome. This drives the groundwater flow toward the salt dome and initiates the uprising circulation of brine within the neighbouring sediments.

**Temperature disturbances and regional flow: Mixed convection**

When an external factor such as head-driven groundwater flow (forced convection) is imposed on a free thermohaline system the resulting regime is referred to as mixed convection (see brief description of driving forces). Here the head level is set equal to the topographic relief so that regional and thermally induced flows occur together. In this section, the results from free thermohaline and mixed convection are compared in order to study the interaction between temperature disturbances and the regional flow.

Temperature and mass distribution resulting from mixed convection (Fig. 5.5.16A-B, respectively) show significant differences with regard to the profile derived from the free thermohaline simulation (Fig. 5.5.14AB). In the mixed convection regime, the thermally induced brine patterns are affected by the regional flow: the short wavelengths of the temperature oscillations characterising the free thermohaline regime (Fig. 5.5.14B) are not preserved in the mixed convection system (Fig. 5.5.16B). The isotherms are shaped by the regional flow: in the recharge areas, the infiltration of cooler water decreases the temperature gradient whereas uprising of warmer plumes occurs in relation to the discharge areas. As a result, the narrow salty fingers observed in the free thermohaline regime (Fig. 5.5.14A) evolve into a smaller number of larger brine plumes which reach the surface at the discharge areas (Fig. 5.5.16A). The brine patterns display a truncated profile in direct relation to the downward flow of freshwater.

Clearly, temperature disturbances and regional flow strongly interact. This interaction can modify the geo-
thermal field and therefore thermally-induced flow. Precisely, decreased concentration and temperature gradients occur in relation to inflow of freshwater while thermally-induced brines are advected toward discharge areas.

Importance of salt-induced temperature disturbances in controlling deep groundwater transport processes. Here the geothermal gradient of the upper crust in the NEGB has been excluded from the simulations. This simulation allows us to demonstrate how important salt-induced temperature disturbances are in controlling transport processes.

Figure 5.5.17 illustrates the resulting mass patterns at the end of the simulation run.

Within the whole Buntsandstein unit the concentration values range from 200 g/L at its surface to 345 g/L, which is the halite fluid saturation, at the top salt. Above the Muschelkalk, dissolved halite flows in the neighbourhood of salt domes. Layered brine plumes spread at both sides of the salt diapirs and do not stretch vertically. The salt dome environment is hydrochemically unique, i.e., groundwater is subjected to large lateral salinity gradients. Along salt dome flanks the density gradient drives...
groundwater flow laterally into the basin. The dissolved halite spreads away from salt bodies by diffusion and rapidly increases the salinity of the pore water throughout the sediments. The resulting brine plumes extend over 30 km in lateral direction. As a result, dissolved halite concentration around salt domes increases with depth. Above salt diapir crests, brackish water with 1 g/L of dissolved salt can reach a depth of between one and half a kilometre. Away from salt domes, the salty plumes do not develop as is the case in the central and eastern part of the basin.

The temperature disturbances illustrated so far were generated for deep salt diapirs. However, salt diapir crests are often close to the surface. Steep salt diapirs close to the basin surface provide a source of high salinity for shallow groundwater which can affect the temperature oscillations. In the next section, a numerical simulation will provide new insights into the effects of temperature disturbances on groundwater transport processes in a shallow salt diapir environment.

**Temperature disturbances and groundwater transport processes in a shallow salt diapir environment**

The temperature field calculated from a coupled fluid flow and heat transport simulation is illustrated in figure 5.5.18. This structural profile includes a steep salt diapir piercing the sediments up to the surface. Different regimes developed within the profile.

Within the salt unit, the thermal regime is conductive. Owing to the strong contrast between the thermal conductivity of the salt and the neighbouring sediments, concave isotherms are found within the salt diapir while convex isotherms are found adjacent to the salt flank.

Above the salt, advective, convective and conductive heat flow affect the whole profile. Within the post-Palaeogene units, the regional flow is dominant. Increased temperature gradients are found in direct association with discharge areas. For instance, the fluid temperature within the Quaternary channel increases by about 2 °C. A similar temperature increase can be observed at the discharge area of the Hemmelsdorf Basin. On the other hand, inflow of cooler water decreases the temperature in the recharge areas.

According to the Rayleigh theory in a porous media, the onset of multi-cellular convection is favoured in thick and permeable units (Nield 1968). This is the case for the Palaeogene and the Cretaceous units where a thermally induced convective regime controls the flow. Thermal plumes of 1.5 km height rise vertically from the Cretaceous basin up to the surface, bounded by the regional flow. A zoom of an ascending thermal plume is shown in figure 5.5.18B. The cell radius is 1 km and the flow rate in the central part of the plume is few millimetres per day. In the deeper units the isotherms are not perturbed and the regime is conductive. Temperature and salinity profiles are shown in figure 5.5.19.

Highly saline brines protruding from the salt diapir into the Cretaceous overwhelm the less intense thermal convective regime. Heat plumes do not stretch vertically but develop almost horizontally in the brine flow direction (compare Fig. 5.5.19 and 5.5.18). Therefore, the temperature gradient increases horizontally from the salt flank toward the center of the profile. As a result, the temperature field can undergo several inversions with increasing depth in the western part of the profile.

In the Eastern part of the basin, thermohaline convection persists within the upper units. Above the horizon-
tally stretched plume, the temperature oscillations generate small convective brine cells (half kilometre radius). As a result, thermally driven saline waters ascend up to the shallow aquifer and spread locally at several points of the surface.

On the other hand, in the other units of the profile, the geothermal gradient do not significantly influence brine patterns as explained in details in Magri et al. (in print).

In summary, the numerical models have shown that thermally-induced flow is an important process in salt-bearing basins, and strongly controls both temperature and concentration gradients. Owing to the presence of thick salt structures, the geothermal field is disturbed. The salt-induced thermal disturbances in turn induce convection of deep brines. However, it is not the only process. Topography-driven flow also influences the geothermal field and can significantly contribute to brine migration. Whereas the principal effects of thermohaline convection could be shown, much more detailed knowledge of transport properties (hydraulic permeability, thermal conductivity) and their regional distribution, including faults and fractures, are necessary in order to achieve more accurate large-scale models.