
Review: Deep groundwater research with focus on Germany

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Abstract While research focuses mainly on the intensively used shallower aquifers, only a little research has addressed groundwater movement in deeper aquifers. This is mainly because of the negligible relevance of deep groundwater for daily usage and the great efforts and high costs associated with its access. In the last few decades, the discussion about deep geological final repositories for radioactive waste has generated strong demand for the investigation and characterization of deep-lying aquifers. Other utilizations of the deeper underground have been added to the discussion: the use of geothermal energy, potential CO₂ storage, and sources of potable water as an alternative to the geogenic or anthropogenic contaminated shallow aquifers. As a consequence, the fast growing requirement for knowledge and understanding of these dynamic systems has spurred the research on deep groundwater systems and accordingly the development of suitable test methods, which currently show considerable limitations. This review provides an overview of the history of deep groundwater research. Deep groundwater flow and research in the main hydrogeological units is presented based on six projects and the methods used. The

study focuses on Germany and two other locations in Europe.

Keywords History of hydrogeology · Groundwater flow · Radioactive waste repositories · Equipment/field techniques · Germany

Introduction

Deep groundwater has been underrepresented in hydrogeological sciences research for a long time and accordingly little is known about its behaviour. Evolution of the term “deep groundwater” is strongly related to the development of the early groundwater sciences in the middle of the nineteenth century. Its meaning has changed from the more speculative and static image as “deep stagnant water” (Weithofer 1936) to a more dynamic understanding. Now, deep groundwater is not only defined by its depth, but by its genesis, age, chemical composition, etc. (Einsele et al. 1983). It is now widely accepted that deeper aquifers are dynamic systems, which are influenced by both surface processes (from the meteoric cycle) and crustal processes (from the lithosphere). Intensive research has mainly focused on characterization of the commonly used shallower aquifers. Great efforts by hydrogeologists have led to a thorough understanding of regional groundwater systems, their driving forces and their hydrochemical dynamics (e.g. Hubbert 1940; Back 1960; Tóth 1962, 1963; Freeze and Witherspoon 1967). The range of research activities is extending from regional-scale basin modeling down to micro-scale laboratory experiments. Complex processes in groundwater systems have been intensively examined in the past and more recently (e.g. Back 1960; Hölting 1969; Stober 1986; Grenthe et al. 1992; Bethke et al. 2000; Magri et al. 2005). The basic groundwater flow concepts in basins are widely accepted, the importance of redox reactions on groundwater quality is well-known, and recently it has become common to compile numerical flow and mass transfer models for the future development of catchment areas influenced by changing boundary conditions caused by climate change. The appearance of new emerging contaminants of concern, the remediation of polluted sites, and the development of new mathematical approaches to describe mass transfer of organic substances in groundwater has been the aim of recent and past

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hydrogeological sciences. There has been less focus on deep aquifers because of their very complex nature, expensive access and negligible importance for supply with respect to potable and irrigation uses.

Except for some deep drilling projects, which have mainly focused on crustal processes, very little research has been performed in the field of deep groundwater flow. However, already these few previous experiments have revealed that the traditional image of stagnant or very slow flowing groundwater with poor hydraulic connection at greater depths seems to be obsolete, e.g. KTB (Kontinentales Tiefbohrprogramm der Bundesrepublik Deutschland [The German Continental Deep Drilling

Program]; see Fig. 1c), and Kola superdeep well in Russia. Simultaneously, interest in deep groundwater research has increased for economic reasons in the last few years. Deep-lying aquifers have become important resources (e.g. for the production of geothermal energy or as an alternative potable water source), or are intended as a medium for final repository (e.g. CO₂ storage). The behaviour of deep groundwater as a transport medium for dissolved substances is an important factor in risk assessment for the worldwide planned or projected final geological repositories for toxic or radioactive waste. A thorough understanding of deep groundwater systems is crucial in the supply of engineered solutions for these

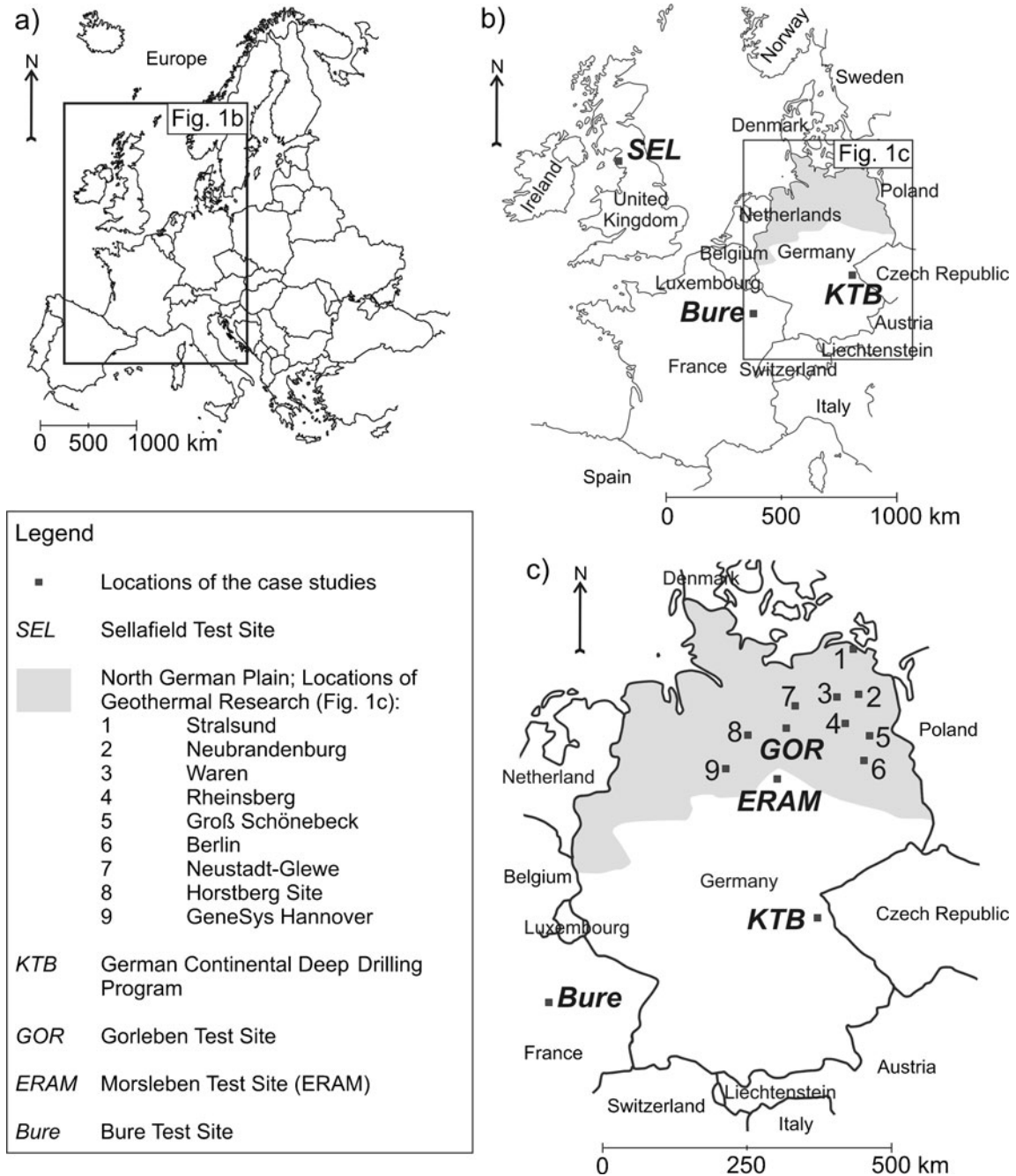


Fig. 1 a–c Locations of the case studies in Central Europe and the UK

modern society requirements. Nevertheless, the knowledge about deep groundwater is relatively poor. Due to their different intentions, the knowledge and experiences acquired during the few experiments that have been conducted so far are widely spread and access to the studies have been time consuming. Research using adapted or newly developed methods shows some limitations caused by the conditions in the deeper underground. The evolution of deep groundwater, its movement, and its chemical behaviour are unclear.

In this paper, previous deep groundwater flow concepts, knowledge about deep groundwater flow in different hydrogeological units, methods, and examples of past and recent research projects (with the main focus on Central Europe and especially Germany; see Fig. 1) are outlined. The aim of this review is to provide a general overview of the history of deep groundwater research and state-of-the-art techniques.

A short history of deep groundwater concepts

Interest in deep groundwater increased in the nineteenth century. One of the main questions was (and still is): Is deep groundwater in motion or stagnant? At that time several authors published their ideas regarding the origin of mineral resources in dike outcrops and in highly mineralized springs. They imagined convection cells forced by gravity-driven descent and heat-driven ascension with the accumulation of mineral resources in dikes (e.g. Beaumont 1850; Cotta 1850; Daubrée and Gurlt 1880; Müller 1860). Other authors believed that the deeper groundwater is connate (from sedimentation), juvenile (from magmatic segregation), or a mix of both (e.g. Behrend and Berg 1927; Weithofer 1936). According to these rules deep stagnant groundwater would prevent the penetration of younger, meteoric water from the surface because of its greater density. Weithofer (1936) introduced a term translatable as “deep stagnant water” (*Tiefenstandwasser*). The deep stagnant water is located below the deepest possible discharge area (which is the ocean). He postulated that due to the friction of moving water within an aquifer, motion of groundwater against gravitation is impossible without outer forces. Above this deep stagnant water, he defines the shallow “flowing water” (*Fließwasser*), which is moving as a part of the meteoric water cycle from its recharge to its discharge area forced by gravitation (accordingly always downgradient). Due to the lack of data from deep wells, the early research was more speculation than interpretation. With the increasing worldwide demand for mineral resources and hydrocarbons during the first half of the twentieth century knowledge of the deeper underground increased. Important contributions to the understanding of regional groundwater flow were given by Hubbert (1940), who introduced modern physics to groundwater sciences. He discussed several existing concepts of groundwater flow from his point of view as a geologist and as a physicist (Anderson 2008). Important for the understanding of groundwater flow was his negation of the concept of deep stagnant groundwater caused by friction.

He showed that the amount of work required to drive a unit of mass of the fluid from one equipotential surface to another is always the same, independent from the flowpath. The consequences for the analytical solution of groundwater flow systems were crucial. One of them is that in a homogeneous aquifer a zone of stagnant groundwater cannot exist (except for groundwater with a considerably different density). Tóth (1962, 1963) applied these essential findings in his analysis of groundwater flow in small basins in Alberta, Canada, by defining boundary conditions like an impermeable lower layer and varying the ratio of basin depth to its lateral extent. The results of his analytical solution were the differentiation of (1) a homogeneous aquifer in shallow zones (local flow systems) with high groundwater flow velocities and relatively large recharge areas, and (2) deep zones (regional flow systems) with very low groundwater flow velocities and relatively small recharge areas. Important conclusions of this work were: (1) regional groundwater flow systems are always dynamic systems with changing local flow systems; (2) the vertical extension of local flow systems depends on the topography; (3) the groundwater flow velocities become lower with depth; and (4) the mineralization of groundwater increases with its depth (according to its velocity within the aquifer). Freeze and Witherspoon (1967) improved and enhanced the analytical model of Tóth (1963) by including different cases of heterogeneity and anisotropy in a finite difference model. They provided useful schemata for different groundwater flow systems and demonstrated the growing prospects and significance of numeric modeling for the solution of hydraulic problems.

In the 1960s the hydrochemical description of groundwater flow systems became more and more important: Back (1960) applied trilinear Piper diagrams to describe different types of groundwater from a coastal basin in the eastern USA. By using the distribution of the different ion concentrations within the Piper diagram, it became possible to describe the genesis of a regional groundwater system. Therefore, he linked the geochemical observations to regional groundwater flow and defined the hydrochemical facies concept (Glynn and Plummer 2005). Hölting (1969) presented a summary of definitions of the term deep groundwater with a focus on the special situation in the North German Basin. He defined deep groundwater, besides its absence from the meteoric water cycle, by chemical attributes. He differentiated the groundwater in northern Germany by its mineralization (deep groundwater shows high salinization) and by its anion ratios. According to Hölting (1969) shallow groundwater is characterized by a high content of hydrogen carbonate and is part of the active meteoric water cycle. He set the depth of this zone at approximately 300 m below the ground surface in the North German Basin. Beneath the shallow groundwater zone he defined a transition zone with increasing sulfate and chloride contents. At depths below about 600 m, a zone of very low groundwater exchange is expected (which he called the “zone of stagnant water with strongly decelerated groundwater motion”). This zone is characterized by high mineralization and high contents of calcium chloride and sodium chloride.

Einsele et al. (1983) presented a comprehensive compilation about the field of deep groundwater research published by DVWK (Deutscher Verband für Wasserwirtschaft und Kulturbau e.V. [The German Association for Water Management and Land Improvement]). In these guidelines, the generally accepted characteristics of deep groundwater were summarized. According to that compilation, the term deep groundwater is not bound to a defined depth below the surface, but to specific characteristics: “‘Deep groundwater’ in Central Europe is defined as water which *originates* from slowly-circulating, deep-lying, subsurface aquifers, although in discharge areas it can occur at relatively shallow depths. It is usually devoid of ^3H and has low ^{14}C values.” (Einsele et al. 1983, p. XIII). The guidelines suggest use of the hydrochemical facies concept (e.g. Back 1960; Hölting 1969) to describe and classify groundwater and its evolution. The increasing impact of isotope dating (by radioactive isotopes) and the evaluation of the paleoclimatic conditions (by stable isotopes) at that time were described. The challenges related to the geothermic gradient (change of density, change of viscosity, heat driven convection) were outlined.

In the second part of the twentieth century an integrated approach for the analysis of specific basins was established, which used all the different fundamental findings and methods for the deep groundwater flow analysis: the development of a regional groundwater flow concept, hydrochemical interpretation, modeling of paleoclimatic with isotopic analysis, and numerical modeling of hydraulic behavior, mass transport, and heat transport. Today, it is accepted that in regional basins, deep groundwater is never stagnant, but moving with very slow velocity towards its discharge area. Certainly stagnant groundwater appears in small isolated aquifers comparable to hydrocarbon traps.

Recently, groundwater research has been in the phase of application, enhancement, and adaptation of the models and methods for the investigation and description of specific basins and deep groundwater flow systems. Seiler (1983) examined the influence of pumping tests on deep groundwater flow. He pointed out that the higher density and temperature of deeper groundwater can lead to inconsistent results. Additionally, he reported on the extreme periods (months to years) needed to reach steady-state conditions during and after pumping tests. Grenthe et al. (1992) investigated the accuracy of redox measurements in deep boreholes. Bethke et al. (2000) compared different transport models (velocity after Darcy’s Law, piston flow, transport of atmospheric ^{36}Cl , transport of geogenic ^4He) for deep groundwater flow in sedimentary basins and emphasized the uncertainties of the term groundwater “age”. The modeling results of an area in the eastern part of the North German Basin by Magri et al. (2005) suggest a slow (1-2 km per 10,000 years) thermally induced free convection, which causes saline springs at the surface. Deep groundwater circulation in crystalline rocks has had more research focus since the 1980s. Research projects about the origin

and behavior of groundwater in the deep crystalline rock basement of southern Germany were published by Lippmann et al. (2005); Lodemann (1993); Lodemann et al. (1998); Stober (1986); Stober and Bucher (1999a, b, 2005, 2007). These authors investigated deep groundwater movement in the Black Forest region (about 1,000 m to maximum 3,500 m depth) and in the Oberpfalz region (KTB: 2–9 km depth). Further examples of deep groundwater research in basins in Germany include Hofmann (1990; Lower Franconia); Schubert (1996; Molasse Basin), and both Naumann (2000) and Magri et al. (2009b) about salty groundwater flow in the North German Basin.

What are the reasons for deep groundwater research?

Considering the wide variety of (mostly ambiguous) definitions of the term deep groundwater in history it becomes clear that the main feature of deep groundwater is its uselessness for daily human consumption and utilization. Interest in the deeper underground and groundwater has increased only with respect to resources, since the beginning of industrialization and especially at the end of the nineteenth century. In addition to the generally increasing scientific interest in evolution of Earth at that time, the main interest in Central Europe concentrated on understanding the origins of mineral resources, ore dikes, and mineralized springs. Since that time, the need to understand the “system earth”, and accordingly regional groundwater systems, has increased significantly. The driving forces were always the prospecting and exploration of resources. One of the most important research fields is the use of geothermal energy, which requires large amounts of hot groundwater. As part of the investigation of potential host rocks for the final repository of toxic, dangerous, or radioactive waste, research on associated deep aquifers is a crucial aspect of safety assessment. The deposition of brines in deep aquifers (as practised for some time in central Germany) strongly affects the groundwater systems and leads to contamination even of the shallow aquifers. An important field of research of deep groundwater is the storage of CO_2 in deep aquifers. For that, utilization of deep groundwater itself should act as the supporting medium for safe and long-term storage. Now, in some regions, deeper aquifers are considered as potential alternatives to shallower, contaminated aquifers. For example, Shibasaki et al. (2007) and Michael and Voss (2008) investigated the potential use of an underlying aquifer for drinking-water supply instead of the arsenic-contaminated shallow aquifer of Bangladesh.

Deep groundwater flow in different geological units

In Germany and Central Europe, the regional hydrogeological formations and the resulting usability of

groundwater for drinking-water supply are quite variable. Accordingly, the knowledge about shallow and deep groundwater flow is quite different depending on the different geologic formations. The most productive and consequently the best known groundwater reservoirs are porous aquifers, like the most important hydrogeological formation, the North German Basin (geographic name is North German Plain). This was formed by glaciers, which overrun northern Germany several times during the Ice Age. The North German Basin is built up by unconsolidated Quaternary sediments, which form multiaquifer formations. The several-hundred-metres-thick aquifers are intensely used for drinking-water supply. For example in the cities of Berlin and Hamburg production wells are pumping at depths between 30 and 430 m below ground surface (Berliner Wasserbetriebe [Berlin Waterworks] 2009; Hamburger Wasserwerke [Hamburg Waterworks] 2010). These deeper aquifers provide enough good quality groundwater for drinking-water supply for altogether about 5.4 million citizens in the both cities.

There are serious problems with saltwater intrusion at the coasts, near salt domes, and in deep aquifers (BGR 2009; Henningsen and Katzung 2002). Because of the occurrence of saltwater at relatively shallow depths, very little research on deep groundwater systems of coastal aquifers has been conducted so far.

Further important sedimentary groundwater storage units in central and southern Germany are the Molasse, the Oberrheingraben (Upper Rhine Graben), and the Niederrheinische Bucht (BGR 2009; Henningsen and Katzung 2002). Because of the availability of sufficient amounts of groundwater with good to excellent quality, and cost-effective pumping from shallow aquifers, it is not common to pump groundwater from deep aquifers.

In the low mountain ranges in the central and southern part of Germany, the productivity and usability of the aquifers depend on the geological setting. In the escarpments of southern Germany (Fränkischer and Schwäbischer Jura), which are built up by limestones, regional karst formations can provide very productive aquifers. In the Pfälzer Wald, Schwarzwald (Black Forest), Spessart and Solling, which are built up by thick sandstones, and in the Vogelsberg (basalt), fissured regional rock aquifers are very productive. Groundwater use in these regions is related to vulnerable karst and fissured rock aquifers, which are at risk from anthropogenic contamination caused by short flow times. Other low mountain ranges, like Harz, Rheinisches Schiefergebirge (Rhenish Slate Mountains), Thüringer Wald (Thuringian Forest), Bayerischer Wald (Bavarian Forest), Erzgebirge and Hochschwarzwald, are predominantly built up by very low permeable rocks, like argillaceous shale, and metamorphic or plutonic rocks. In these areas, only local aquifers built up by unconsolidated Quaternary sediments in river valleys are usable for drinking-water supply. There, the common source for potable water is surface water (BGR 2009; Henningsen and Katzung 2002).

Sedimentary basins

The largest and most important sedimentary basin in Germany, the North German Basin, is composed of Tertiary and Quaternary glacial sediments, which are underlain by Palaeozoic and Mesozoic sediments up to a maximum depth of about 10 km. In the basin, the shallow freshwater aquifer is separated from the underlying saltwater aquifer by the Tertiary Rupel Clay. This clay barrier lies at a depth of several tens of meters to some hundreds of meters. Due to the easy supply of large amounts of excellent quality groundwater from the shallow aquifer, only a little was known about the deeper salty aquifer and the underlying basement. This situation has changed with the beginning of deep exploration programs for hydrocarbons and geothermal research. In general, groundwater becomes more mineralized with increasing depth in the North German Basin (Hölting 1969). The increasing mineralization is probably caused by the dissolution of evaporates from the Zechstein formations (mainly from large salt structures). Evidence for this comes from Naumann (2000), who compared the geochemical analyses of five geothermal boreholes at depths between 1,250 and 3,250 m in northern Germany. Magri et al. (2005) modeled very slow but deep-reaching thermally induced convective flow, which causes transport of brine to the surface (salty springs). Highly mineralized aquifers, caused by dissolution of evaporates, are often observed.

In coastal aquifers high salinity is caused by connate seawater (as a residue from a former marine sedimentation) or by mixing of intruded seawater and evaporate-mineralized meteoric water. An example of a coastal sedimentary basin is the Sellafield groundwater system in northwestern England (United Kingdom), which contains waters of three levels of salinity (fresh, saline, and brine; Black and Brightman 1996). An important controlling factor of coastal basins is the location and the evolution of the saltwater–freshwater interface, which has a crucial impact on the groundwater flow system (Masterson and Garabedian 2007; Werner and Simmons 2009).

In general, groundwater flow systems of regional sedimentary basins are topographically driven and Darcy flow can be assumed. Nevertheless, in large sedimentary basins, isolated zones of stagnant or very old groundwater are reported (e.g. the Dogger aquifer in the Paris Basin, France; Marty et al. 2003). Therefore the Darcy flow model is, maybe, not always the best flow model for deep and slow groundwater movement (Bethke et al. 2000).

Igneous and metamorphic rocks

Igneous and metamorphic rocks cover wide areas of Germany. Most of these rocks were generated during the Precambrian and the Palaeozoic Age. In many regions, extensive mining was conducted in the past. The mountain range Erzgebirge, in particular, has a long mining tradition for ore, silver, uranium, and other mineral resources (Henningsen and Katzung 2002). Only a little is known about the deep groundwater flow behaviour in crystalline

basement. Crystalline rocks themselves exhibit very low permeability, are nearly insoluble and highly rigid, and exhibit low sensitivity to high temperature (BGR 2007). Larger crystalline rock formations are fissured by tectonic stress or by expansion during their ascension. Because of the enormous overburden pressure, researchers used to assume that no groundwater flows in these fissures at great depths. These days, it is accepted that at great depths groundwater may flow and even circulates (Rybach 1997; Smithson et al. 2000). Carlé (1975) explained mineral springs and thermal waters in the crystalline basement of the Black Forest with the mixing of different groundwater flow systems. Stober (1995) enhanced this work by adapting the model of topography-driven flow to the Black Forest region. Pumping tests show that strongly fissured granitic rocks may behave as homogeneous and isotropic aquifers. Stober and Bucher (2007) reported on hydraulic conductivities up to 10^{-6} m s^{-1} at depths of about 1 km. From the Kola well, which was drilled to about 12 km into the crystalline basement of the Kola Peninsula, fissure-related water was reported (Kremenetsky and Ovchinnikov 1986; Popov et al. 1999). Rybach (2009) used geothermal data to evaluate the deep groundwater flow characteristics of three example sites in the Hercynian basement of Western Europe (at various depths from 1.5 km to 5 km). For all sites he found similar ranges for very slow groundwater movements of 10^{-10} to $10^{-11} \text{ m s}^{-1}$ within a depth range of groundwater circulation of $\sim 5\text{--}7$ km. According to the findings of a pumping test in the 4,000 m pilot hole of KTB, Stober and Bucher (2005) concluded that “the water-saturated fracture pore space of the brittle upper crust is highly connected, hence, the continental upper crust is an aquifer”. Accordingly, large areas without fissures and cracks were not expected to be found in the crystalline rocks of Germany. The German Federal Institute for Geosciences and Natural Resources (Bundesanstalt für Geowissenschaften und Rohstoffe, BGR) concluded that it is unlikely to find potential suitable host rocks for final repository within crystalline rocks in Germany (BGR 2007).

Rock salt

Rock salt formations were mined for more than 100 years in Germany. Extensive knowledge about the behaviour and properties of these formations exists (BGR 2007). The most important salt formation in Germany is the Zechstein salt formation, which was deposited at the end of the Permian Age. The Zechstein salt formation is composed by seven evaporate cycles, each of them containing carbonates, gypsum, anhydrite, rock salt, potash salt, and argillaceous rocks. The ductile behaviour of rock salt and the release of tectonic stress lead to the ascension of the Zechstein formation through the overburden sediments at many locations. More than 200 of the resulting salt structures (salt domes, walls, and pillows) occur in the North German Basin. They accumulate very important mineral resources such as potash and rock salt, and, in

traps on the structure flanks, petroleum and natural gas (Henningsen and Katzung 2002). Rock salt is quasi-impermeable to fluids and gases (e.g. Baumann et al. 1995; BGR 2007). Within a salt dome, only connate water from its formation during the Zechstein and pore water originating from mineral metamorphosis exist (e.g. the release of up to six water molecules from one carnallite molecule at temperatures exceeding 85°C). Although no moving groundwater is expected within a salt structure, a salt dome affects the regional groundwater flow system. By subsrosion, which means the dissolution of salt by groundwater, a freshwater–saltwater system will be established. Consequentially a low permeability cap rock will be formed by the remaining residues (gypsum, anhydrite, clay minerals) at the top of salt domes. At the flanks of the salt dome a quasi-stationary equilibrium will be established. Its high mineralization and the resulting higher density causes very slow groundwater movement. Probably, gravity-driven groundwater flow can cause convection cells (Magri et al. 2009a, b). Anyway, in the overburden sediments highly mineralized groundwater has often been reported even at the surface, caused by groundwater circulation (e.g. Langkutsch et al. 1998). A further attribute of rock salt is its very good thermal conductivity. The combination of the rock salt properties (impermeability, heat conductivity, ductile behaviour) lead to the recommendation, even in 1963 (BGR 2007), of rock salt as the favoured host rock for high level radioactive waste (Röthemeyer 1991).

Argil/argillaceous rocks

Argil and argillaceous rocks were deposited in many different stratigraphic formations within several sedimentary basins in Germany. The different conditions during sedimentation caused strong variations in thickness, distribution, homogeneity, and formation. The maximum thicknesses of clay formations were reached in great basins (North German Basin; Molasse Basin at the foothills of the Alps). The main clay formations were deposited during the Jura, the Lower Cretaceous, and the Tertiary ages. The most important formation in northern Germany is the Rupel Clay (Tertiary), mentioned previously, which divides a lower saltwater aquifer from an upper freshwater aquifer in many areas. In southern Germany, the Opalinus Clay (Jura) accumulates an important argillaceous rock formation. Clay or argil will not be extracted by underground mining, but by open pit mining. There are no experiences about the behaviour (e.g. mechanical strength, thermal conductivity, etc.) of deep clay formations comparable with the knowledge about salt formations in Germany (Hoth et al. 2007). Because of the impermeable properties of argil formations, they act as an aquitard. They protect an aquifer that is in use for drinking-water supply, from groundwater contamination (from the surface) or groundwater salinization (from the underlying layers). At higher levels of diagenesis the sealing properties of clay decline, caused by the appearance of micro-fissures and micro-cracks. Because of the many different formations of argillaceous rocks, a general estimation about its stability

at great depths is not possible (BGR 2007; Czaikowski et al. 2005; Hoth et al. 2007). According to the experiences of the petroleum industry, argillaceous rocks reach their greatest impermeability at depths between 400 and 600 m (Hoth et al. 2007). The main groundwater research related to argillaceous rock formations is focused on the aquifer formations surrounding potential host rock clay. In argil and argillaceous rocks, mass transport occurs, which is driven by thermodynamic forces as near-field transport (thermo-osmosis, thermo-diffusion; Horseman and McEwen 1996). Clay formations can be overpressured or underpressured compared with the surrounding aquifers depending on their geological history of subsidence. This leads to groundwater flowing out of the formation or into the formation and may change the existing flow system (Houben 2006; Raven et al. 1992). Armstrong et al. (1998) reported on the influence of clay-water ion exchange on the pore-water chemistry of the surrounding aquifers. With increasing depth, the temperature increases, which leads to clay mineral metamorphosis at temperatures higher than 100°C (BGR 2007). Horseman and McEwen (1996) pointed out that higher temperatures (e.g. by geological sinking or by a high-level radioactive waste repository) may lead to high pore pressures in low permeability rocks. Accordingly, the permeability of argil will be increased by fissures because of shrinkage under increasing temperatures. Mazurek et al. (1998) reported variable transmissivities within a system of faults. A further important property of clay minerals is their high sorption potential, which is an interesting attribute for the research on all kinds of final repositories (Hoth et al. 2007).

Selected case studies of deep groundwater research

A collection of six projects in different geological settings is presented, which is an overview of the various objectives and approaches in the field of deep groundwater research. Two of the six case studies are not located in Germany, but in England (UK) and France. These projects were chosen for this review because of their exemplarity with respect to deep groundwater research in their respective geological settings.

Sedimentary basins: the Sellafield Test Site

The Sellafield Test Site is located in north-western England near the Irish Sea (Fig. 1b). Starting in 1991, an extensive investigation program was conducted by NIREX (originally known as the Nuclear Industry Radioactive Waste Executive) to test the site as a potential final repository of radioactive waste produced by the UK. Therefore, the Sellafield area is a very well analyzed coastal basin (Bath et al. 2006). The geological investigations of the basin included the drilling of 20 deep boreholes, seismic surveys, and airborne geophysical surveys. The basin is filled with Permo-Triassic sedimentary rocks, which are underlain by Ordovician metavolcanic basement

(Chaplow 1996). The sedimentary rocks are mainly composed of sandstones (Sherwood Sandstone Group), which form a locally important aquifer with a thickness up to 500 m. The underlying basement consists of metamorphosed ignimbrite (Borrowdale Volcanic Group), which is a low permeability fractured aquifer (Bath et al. 2003; Chaplow 1996). Because of their low permeability, the basement rocks were intended as the potential host rock for the UK's final repository (Bath et al. 2006). Therefore, the identification of hydrogeologically significant fractures is crucial in the fracture-flow-dominated Borrowdale Volcanic Group (Chaplow 1996). For understanding of the hydraulic behaviour of the individual geological and hydrogeological formations, the geometry of all observable fractures on the different outcrops was mapped in detail and fractal concepts were applied. Therefore, for some formations (Mercia Mudstone Group) only a little direct information on the hydraulic properties is available because of the lack of outcrops in the Sellafield area (Michie 1996). For understanding the flow of deep groundwater between sedimentary and crystalline formations and to derive a conceptual model of the regional hydraulic system, deep boreholes were drilled along profiles several kilometres long and from a maximum depth of 1,950 m (Bath et al. 2006; Black and Brightman 1996; Metcalfe et al. 2007). Production tests were conducted over the full length of the boreholes. Due to the low flow, the zones of hydrogeologically significant fractures could not be identified by spinner logging, but only by temperature and conductivity logging (Chaplow 1996). Permeabilities of the overlying Sherwood Sandstone Group were measured, although on core samples measured values are several orders of magnitude less than those obtained during borehole pumping tests, observed as field permeability (Michie 1996). Using the acquired data about the fracture system from the outcrops and the borehole studies, a discrete fracture network model was established by using NAPSAC, the finite-element software package for groundwater flow and transport in fractured rock (Hitchmough et al. 2007). Although the fracture modelling was consistent with the observed variability of heads, the authors emphasized that more than one fracturing concept will be consistent with the observed data (Heathcote et al. 1996). Groundwater samples were taken from the boreholes, which was difficult because of the small permeabilities of the Borrowdale Volcanic Group and because of the influence of the drilling fluid on the groundwater samples. Although groundwater samples were obtained during 163 borehole tests, only 79 samples showed less than 10% contamination by drilling fluid. Even these samples could not be used to measure reliable pH, HCO_3^- , ^{14}C , and ^{13}C values. Especially the weak ^{14}C data made it very difficult to date the groundwater (Bath et al. 2006).

The gained knowledge about the fracture system was combined with the determined hydrogeological parameters and with attributes derived from cross-hole seismic tomography and vertical seismic profiles (Michie 1996). Three regimes were defined for the Sellafield Test Site by Black and Brightman (1996) to establish the conceptual hydrogeological model: (1) Coastal Plain Regime

(freshwater system, which is topographically driven and related to present day precipitation); (2) Hills and Basement Regime (mixture of freshwater from precipitation and saline groundwater of different origins, which is mainly topographically driven and at depth driven by density variations); and (3) Irish Sea Basin Regime (basin-derived brines, which are driven by basin processes over long periods of time). The groundwater system in the sedimentary cover rocks and basement formations consists of water with different origins, ages and salinities. The oldest groundwater was detected in off-shore sedimentary rocks. It was probably meteorically recharged more than 2 million years ago. The saline water in the basement formation was recharged between 10,000 years and 2 million years ago. The stable oxygen and hydrogen isotopic compositions suggest a dominantly meteoric origin of all water types (Bath et al. 2006). Based on the conceptual hydrogeological model, several numerical models were tested with respect to various features such as porosity and fracture flow, complex geology, anisotropic formations, and the presence of dense solutes from more than one source. A two-dimensional (2D) model was set up (Heathcote et al. 1996) to identify recharge and discharge areas and to constrain the hydraulic conductivity of the sandstone (model features: porous medium, steady-state, 2D-flow, only topography-driven force); the codes used were MODFLOW (a modular finite-difference three-dimensional groundwater flow model) and NAMMU (a finite-element software package for groundwater flow and transport modelling in porous media). 2D-vertical-section density dependent models were set up (Heathcote et al. 1996; model features: included basement, anisotropy, topography-driven and density-driven flow); the code used was SUTRA (a saturated and/or unsaturated, constant or variable-density fluid flow model, for solute or energy transport). By establishing a 3D-model (Heathcote et al. 1996) using simplified geology, the interaction of salinity and geology, and the evolution of pressures and salinities could be demonstrated (model features: horizontal layers, faults represented simply by geometrical displacements in a vertical plane, two water layers of different density); the code used was SWIFT (a model to simulate groundwater flow, and heat, brine, and radionuclide transport).

Although the numerical modelling shows good comparability with the observations of salinity and head, certain details remained unexplained (Heathcote et al. 1996). By investigating the paleoclimate, Heathcote and Michie (2004) determined that the Sellafield groundwater system will be affected by major climate changes, particularly by glacial-interglacial cycles (land and sea level changes, erosion, glaciation, and permafrost). The main finding was that the potential repository would be situated in the saline groundwater zone and the flow path from the repository back to the surface environment would be long and directed to the sea (Michie 1998). Anyway, all investigations were stopped by a political decision concerning the site of Sellafield and its scenic value in 1997. Currently, there is no research for a final

repository for radioactive waste in the UK (Bath et al. 2006; Michie 1998).

Sedimentary basins: geothermal research in the North German Plain

Energy and heat generation with geothermal technologies has had a sustained rise in importance in the last few decades. Geothermal research and application started early in the North German Basin because of the locally very capable geological conditions and the policy of self-sufficiency of the former German Democratic Republic (GDR, i.e. East Germany; Seibt and Kellner 2003). The geothermal gradient is relatively low in this sedimentary basin. Accordingly, the geothermal research in northern Germany contributes a significant part to the deep groundwater research in Germany. Already in the 1980s, intensive investigations started by testing production and reinjection wells and equipment. In 1984, a geothermal heating plant for heat supply to a residential area was commissioned in Waren (hot water supply from about 1,500 m depth; Fig. 1c). Further sites were Neustadt-Glewe (2,200 m depth) and Neubrandenburg (1,150 and 1,250 m depth). All of them were located in the German state of Mecklenburg-Western Pomerania. In the meantime, more sites were investigated and developed successfully in the North German Basin. For example, some German Parliament buildings in Berlin such as the Reichstag and some further new buildings, are supplied with water from about 300 m depth (Seibt and Kellner 2003). Because of the high salinities of deep groundwater in the North German Basin (Höiting 1969), it is common to reinject the cooled brine into the aquifer (Frosch et al. 2000; Kühn et al. 2002). The interests of deep groundwater research in the field of geothermal energy supply are related to the prospects of finding widely (lateral) extended productive formations, providing high flow rates, high temperatures, low salinities, and long-term stable production and reinjection rates (Seibt and Kellner 2003). Adequate sandstones (high effective porosity, high permeability, large net thickness, low accumulated matrix, low diagenetic changes) were found in the North German Basin at depths down to about 3,000 m (Hurter and Schellschmidt 2003; Seibt and Kellner 2003).

To generalize, the obtained knowledge from individual projects on geothermal energy, the origin and evolution of the deep groundwater in the North German Basin has to be understood. Naumann (2000) compared deep groundwater samples from five different geothermal boreholes in northern Germany (ranging from 1,250 to 3,250 m depth), as mentioned previously. The results suggest the same origin and evolution of all samples. According to the δD - ^{18}O ratios, the investigated samples are the mixture of a strong meteoric component with some seawater, which took place ~20–50 million years ago in the aquifer (according to the cumulative He-ages). The groundwater of the North German Basin is highly mineralized. The main component is NaCl (up to 200–300 g L⁻¹ total dissolved solids). By interpreting the Br–Cl ratios,

Naumann (2000) assumed that the high salinity is probably not caused by mixing with seawater but by dissolution of Zechstein salt.

One of the aims of geothermal research is the determination of the permeability of the aquifer. The high salinity of deep groundwater in the North German Basin may cause several dissolution and precipitation reactions in the aquifer during continuous extraction and reinjection. This may have an impact on the hydraulic properties of the geothermal reservoir. Therefore, processes such as solution, dissolution, and cementation are often described with chemical models. Because of the great number of possible mineral reactions during pumping and injection within an aquifer, such models become very complex and simplifications have been postulated—e.g. Kühn et al. (2002) examined the hydrothermal sandstone reservoir of Stralsund at the Baltic Sea (Fig. 1c). The target formation (Buntsandstein) is located at depths of about 1,500 m. Since the reinjection of cooled brine into deep aquifers strongly affects the mass and energy flows in the reservoir Kühn et al. (2002) modelled the impact on the aquifer by using the subsurface flow and hydrogeothermal simulation system SHEMAT. For the modelling it was assumed that only calcite and anhydrite would react in the aquifer. They found that the injection of cooler and accordingly more viscous water leads to a reduction of injectivity of the aquifer. This effect will be reduced by thermally induced mineral reactions (by the dissolution of anhydrite). They refer to the difficulty of estimating changes of permeability during modelling of chemical reaction rates, as the permeability not only depends on the porosity, but also on the structure of the pore space. Accordingly, the understanding of pore space changes caused by thermally induced precipitation and dissolution reactions is crucial for the use of geothermal energy (Kühn et al. 2002).

Frosch et al. (2000) investigated the impact of reinjected cold brine on reservoir parameters of deep aquifers. They suggest that the classical reservoir parameters like porosity and permeability are not adequate for the description of the impact of reinjection on the aquifer. For that, they examined the fluid–solid interface and the tortuosity of migration channels in porous media by using nuclear magnetic resonance (NMR) on samples from deep drill cores of the geothermal wells of Neustadt-Glewe, Neubrandenburg, and additionally Rheinsberg (in the German state of Brandenburg). Based on these data, the transport properties of hot and cold fluids in deep aquifers may be better estimated, but laboratory measurements, like those taken during investigations of drill cores by NMR, are limited by scale effects. In Hannover, a research group—GeneSys – Generierte Geothermischen Energiesysteme (artificially generated geothermal systems)—tested the ‘single borehole method’ by reinjecting the cooled brine via the annulus in the same borehole into a more shallow permeable rock formation. Simultaneously the overall low permeability of these formations should be enhanced by hydraulic fracturing. A deep circulation system should be established through the extraction of water from one sandstone layer and reinjection into a

shallower sandstone layer (Kehrer et al. 2007). Ghergut et al. (2009) conducted a single-well inter-layer flow path tracer test in a 4-km-deep former gas exploration well, located north-east of the city of Hannover (Horstberg site). The exploration well was used for preliminary studies for the GeneSys project. The test was conducted between two sandstone layers, which are separated by a few hundred metres of faulted and fractured claystone. By this test, not only the mean residence time of the injected water as it moves towards the production horizon should be determined, but other important aquifer parameters should be determined such as residence time distribution, flow-storage repartition, and transport-effective fracture densities (Ghergut et al. 2009). However, these parameters could not be determined reliably in that test. Because of the short test duration and very low tracer recoveries, the tracer breakthrough curves could not be extrapolated for longer time periods than the test duration itself (Ghergut et al. 2009).

Another current large-scale research project, involving the utilization of deep groundwater systems for the supply of geothermal energy and heat, is located near Groß Schönebeck (German state of Brandenburg). Helmholtz-Zentrum Potsdam – Deutsches GeoForschungsZentrum (Helmholtz Centre Potsdam – German Research Centre for Geosciences) deepened a former gas exploration well down to about 4,300 m to identify suitable geological structures and to develop new methods to increase the productivity of deep geothermal reservoirs. For that, technologies to enhance the permeability of deep aquifers were tested in the well, which serves now as a geothermal in situ laboratory (Huenges and Bruhn 2007). Zimmermann et al. (2009) reported on two different technologies tested in the target formations (Upper Rotliegend sandstones and Lower Rotliegend volcanic rocks). They used high viscous gel and proppants to stimulate the sandstone aquifer by hydraulic fracturing. High flow rate hydraulic fracturing (waterfrac) stimulation was done within the low permeability volcanic rocks. For technical reasons the waterfrac experiment had to be conducted over both formations. Accordingly, it was not possible to assign the success of the stimulation to a single formation, because fracturing occurred in both rock types. The efficiency control of such aquifer enhancement technologies is quite challenging. One simple and common method is the comparison of the water-level lowering during pumping with a specific flowrate before and after treatment (Ghergut et al. 2009). According to that test, the production rate could be increased, but is still too low for the profitable generation of geothermal electricity (Reinicke et al. 2005; Zimmermann et al. 2009). The research on geothermal resources provides some of the most important findings about deep groundwater behaviour. Additionally it will probably be one of the most important utilizations of these systems in the future.

Metamorphic rocks: the German Continental Deep Drilling Program (KTB)

The KTB was a scientific drilling project conducted to study the deeper continental crust. The drilling site is

located in Windischeschenbach in northeastern Bavaria, Germany (Fig. 1c). This location was chosen for its specific geological properties, which were: (1) its location in an important suture zone; (2) the occurrence of gravitational, magnetic, and electrical anomalies; (3) the presence of specific seismic reflectors (which were linked to fracture zones); and (4) a probably relatively low geothermal gradient. The drilling operations of KTB-VB (Vorbohrung; the KTB pilot borehole) started in 1987 and reached about 4,000 m depth. During this pilot phase, which was conducted to determine the technical concept for the main borehole, several important findings were obtained: (1) a higher geothermal gradient than expected; (2) a strong lithological heterogeneity; and (3) significant fluid inflow zones. Afterwards, the KTB-HB (Hauptbohrung; the KTB main borehole) was drilled to a depth of about 9,100 m. The operations were completed in 1994 (Emmermann and Lauterjung 1997). The two boreholes provided samples of fluid inclusions (paleofluids) as well as free fluids in the crystalline basement (Möller et al. 1997). Indeed, hydrochemical sampling showed some limitations caused by the long pumping duration during which the sample water travelled several kilometres up to the surface. This led to oversaturation with respect to calcite, fluorite, chalcedony, and quartz of the sampled fluid (Stober and Bucher 2005). This effect is mainly caused by the strong decrease of fluid temperature during pumping from 119°C down to 11°C at the surface (Lodemann et al. 1998). A further consequence of the long pumping time is diffusive degassing during uplift and accordingly undersaturation and elemental fractionation of noble gases (Lippmann et al. 2005). Möller et al. (1997) reported problems with hydrochemical analysis and interpretation of the samples obtained during a 4-month pumping test in the KTB-VB just after finishing the drilling operations. The borehole had to be stabilized and the used drilling mud, including several organic additives, contaminated the surrounding pore- and fissure water and affected the chemical and isotopic results. Even at the end of the pumping test for determination of several elements and gases, the samples were slightly contaminated with the organic additives. Additionally, heavy metals from abrasion of the drilling equipment were found. The rare earth analysis was affected by the enforced release of these elements during drilling, which altered the rock and mineral surfaces. The concentration of rare earth elements in the drilling fluid further increased during the drilling operations, because of recycling of the fluid (Möller et al. 1997). Möller et al. (2005) reported of a 1-year pumping test on the KTB-VB between 3,850 and 4,000 m depth, which was conducted between 2002 and 2003. Lippmann et al. (2005) measured the concentrations of H₂, O₂, Cl₂, N₂, CH₄, and noble gases during this test. All gas concentrations and isotopic signatures, except those of ²²²Rn, remained constant during the 12 month of pumping. These data and the large fluid flow rates suggest a homogeneous and large fluid reservoir in that depth. Lippmann et al. (2005) conclude that the findings of the 1-year pumping test are more reliable

compared to the 4-month test because of the much lower level of contamination by drilling mud. Stober and Bucher (2007) reported hydraulic conductivities (K) of about 10⁻⁸ m s⁻¹ resulting from the long-time pumping test in the KTB-VB. They conclude possible Darcy flow mechanisms even at great depths, which may provide advective fluid and heat transport. The isotopic and hydrochemical fingerprint suggests that the pumped water is a mixture of ascending basement brine and descending very old meteoric water. Hydraulic tests revealed a communicating system of fractures. Möller et al. (1997) and Rybach (1997) concluded that in deep-lying aquifers, slow but extensive movement of crustal fluids appears. From the findings of the long-time pumping test in the KTB-VB, Stober and Bucher (2005) summarised that the water-saturated fracture pore space of the brittle upper crust is highly connected. This leads to their conclusion that the continental upper crust is an aquifer. Despite all the technical limitations, the KTB project showed at least that Ca–Na–Cl brines associated with gases (N₂, CH₄) occur in open fracture systems at depths below 5.5 km (Lodemann et al. 1998). This is, from the view of a hydrogeologist, a crucial finding.

Rock salt: the Gorleben Test Site

The Gorleben Test Site (Fig. 1c) is located in the north-east of the German state of Lower Saxony, near the River Elbe. The test site will be investigated for its suitability as the German final repository for all kinds of radioactive waste. These investigations are based on the recommendation for salt as the best host rock for final repository by the BGR in 1963 (Röthemeyer 1991). Gorleben was chosen because of its location within a sparsely populated area near the border to the former GDR. Starting in 1979, the Gorleben salt dome was investigated with a geological and hydrogeological exploration program (Klinge et al. 2002). The aim of this program was the description of the regional groundwater flow system and the estimation of the prospective evolution of this system, considering a potential use as a repository. The investigation of the groundwater flow system was conducted between 1979 and 1999 and included (Klinge et al. 2007): the construction of a monitoring network (maximum depth about 450 m), long time running pumping tests, pedological field mapping (for the estimation of percolation rates), geothermal investigations (to indicate the groundwater movement by temperature anomalies), analysis of isotopes and noble gases (to estimate the groundwater age and residence time), and numerical modelling (2D with variable density, 3D with constant density). It is accepted that in a compact salt structure, like a salt dome, no groundwater moves. Therefore, the main focus of hydrogeological research on salt domes is the groundwater flow system at the periphery of the structure. In Gorleben, the most important structure for groundwater flow is the Gorleben Channel (*Gorlebener Rinne*). This was caused by partial glacial erosion of the Tertiary Rupel Clay and the protecting cap rock, which lead to a hydraulic window (Klinge et al. 2002). Accordingly, fresh groundwater from

the upper aquifer is in contact with brines from the dome. A freshwater–saltwater system was established, which leads to slow subsidence of the salt dome by the solution of salt. Röthemeyer (1991) reported a subsidence rate of about 0.025 to 0.062 mm per year. For a better understanding of the groundwater flow system, including the freshwater–saltwater effects and the dimension of subsidence, numeric modelling was conducted. Because of the limited technical capabilities of numerical models at that time, the design of the compiled 3D-model (GS4000, a program code developed by the BGR to simulate 3D groundwater movement in constant-density porous media) could not be taken into account in the late 1980s (Klinge et al. 2007). The area northwards of the River Elbe was strongly simplified in the model because of the lack of data during the compilation of the model (this area was part of the former GDR until 1990). Bearing in mind these limitations of the numeric 3D-model, an average groundwater velocity from the salt dome surface to the biosphere of some thousands up to 17,000 years was calculated. As the density difference between the saltwater and the freshwater zone affects the groundwater flow, a 2D-model (SUTRA) considering variable density was also conducted. The 2D model was started with simple and idealized geometries and parameters. Step by step, more heterogeneities were introduced leading to a more complex model (Klinge et al. 2007; Schelkes et al. 2001). Several models were constructed with different initial conditions to find a salinity distribution comparable to present day conditions. During these simulations, it became clear that steady-state conditions will not be reached but that the past density distribution (e.g. during ice ages) still affects the groundwater system today (Schelkes et al. 2001). Most input parameters for the model were derived by laboratory experiments on rock samples (porosity, permeability, adsorption capacity, and diffusion data). The hydraulic conductivity was estimated with various empirical approaches, which use the grain-size distribution. Field permeabilities, storativity values, and leakage coefficients were determined with single-well pumping tests (“local scale”) and long-term pumping tests (“regional permeabilities”). The long-term pumping tests were used for identification of potential hydraulic connections between different aquifers in the sedimentary cover of the salt dome (Schelkes et al. 1998). Although no connection could be identified, Schelkes et al. (1998) emphasized that this result is no proof for the complete hydraulic isolation of the lower aquifer in terms of contaminant transport over very long periods. Caused by the limited capability of the density dependent 2D-model at that time the findings show some uncertainties. It seems that the groundwater velocity was overestimated by ignoring the density differences in the 3D-model (Klinge et al. 2007). For characterization of the groundwater system the hydrochemistry was investigated. Since the saline water originated from dissolution of the Zechstein rock salt, there are only a few variations in the saline water composition, which limits the significance of chemical and trace element analysis (Schelkes et al. 1998).

In 2000, all research activities in Gorleben were stopped by a decreed moratorium by the government, which caused stagnancy in several investigation projects. As the moratorium ended in October 2010, it has to be decided which research projects, like the numerical modelling project, have to be updated or started again.

Rock salt: the final repository for radioactive waste at Morsleben (ERAM)

ERAM (Endlager für Radioaktive Abfälle Morsleben; see Fig. 1c) is located in the western part of the German state of Saxony-Anhalt as a part of the Allertal salt structure. It was the first regular operating deep geological final repository for radioactive waste worldwide. ERAM also will probably be the first repository worldwide that will be regularly closed and sealed after its working phase. Morsleben was a former commercial salt mine, which was established about the year 1900 (Shaft Bartensleben and Shaft Marie). In 1970, Morsleben was chosen from 10 ancient salt mines by the government of the former GDR as the national final repository for radioactive waste. After the reunion of Germany in 1990, the low and medium radioactive waste of the Federal Republic of Germany (FRG) was stored at Morsleben. Between 1971 and 1998 a total of about 37,000 m³ of low and medium radioactive waste was stored in ERAM (BfS 2009).

The storage of radioactive waste was stopped for legal reasons in 1998. After that, in 1999, the operator of ERAM, the Bundesamt für Strahlenschutz (Federal Office for Radiation Protection; BfS), resigned the further use of ERAM (Brasser and Droste 2008). Due to the natural convergence of salt by rock pressure, selected parts of the mine will be filled by a mixture of salt and cement. By this procedure, the mine layout should be stabilized until the administrative permission for decommissioning is granted. For the final closing, the total deposit area and the shafts will be filled with the salt-cement mixture and sealed. All buildings and constructions above ground will be removed (BfS 2009). It is assumed that the closing phase will take ~10–15 years after the final decommissioning permission has been granted. As part of the administrative procedure for obtaining the permission for decommissioning of a final repository (including licensing procedure, environmental impact assessments, public participation, etc.) the BfS, as the operator, has to prove its long-term safety for the biosphere. For that, an extensive research program was undertaken.

As rock salt is impermeable to water and gas, no groundwater motion within the salt structure is expected at Morsleben. Therefore, the main interest of hydrogeological research at Morsleben is the groundwater flow system at the periphery of the salt structure. Accordingly, the research program focused on the description and quantification of the regional-scale groundwater flow system around the salt dome. For that, a conceptual regional groundwater model was developed, which was used as the base for numeric modelling of groundwater flow and potential dispersion of radionuclides in the cap rock of the

repository. To estimate the model parameters, an extensive hydrogeological research program was conducted. It included several geophysical surveys (e.g. seismic reflection and high-resolution seismic methods). For the estimation of the hydraulic system parameters, pumping tests and core analyses were conducted, along with slug and pulse tests (rapid increasing of the water level and observation of its decline). These tests are relatively cheap, fast, and no water is pumped (which has to be disposed of). As a result, the transmissivity for the whole test interval (varied between 10–150 m within the borehole) is obtained. The resulting permeability (transmissivity divided by length of test interval) represents a mean value and may be of no relevance if the main groundwater flow contribution is from single fractures or fracture zones (Langkutsch et al. 1998). The identification of hydraulically relevant fissures was conducted by fluid logging. The drilling fluid was replaced by fresh water and the water level was decreased by pumping. The low hydraulic conductivity of many investigated formations leads to an often underestimated fracture flow, especially if the water level drop is too small to stimulate flow in the very small fractures (Langkutsch et al. 1998).

A campaign for the estimation of groundwater movement in single boreholes (groundwater monitoring wells) was conducted (radiohydrometric single-borehole method using a radioactive tracer for tracking the groundwater flow direction and velocity in single boreholes; Delakowitz 1996). In these tests, a radioactive substance (^{83}Br) was injected and mixed into packered test intervals of 50 cm within selected groundwater monitoring wells. The decline of the concentration and the direction of the radioactive tracer movement can be measured and was used for estimation of groundwater flow velocity and direction (Langkutsch et al. 1998). A low detection limit ($<0.005 \text{ m day}^{-1}$) was achieved, and explained (Delakowitz 1996) by the impact of molecular diffusion on mass transport at lower groundwater flow velocities. This method, as with all passive single-borehole methods, overestimates the hydraulic parameters (velocity and hydraulic conductivity) of the aquifer. The very high hydraulic conductivity of the borehole compared to the hydraulic conductivity of the aquifer forces the naturally parallel groundwater flowlines towards the well (divergent flow). Accordingly, the velocities obtained by this method overestimate the natural groundwater flow velocities (Delakowitz 1996).

The high-density differences in the groundwater system of Morsleben are relevant for its hydraulic behaviour. Therefore, analysis of the hydrochemical and isotopic parameters in groundwater and pore-water samples from drilling cores was conducted; this aided the determination of salinity, description of the groundwater genesis, dating by noble gases analysis, and estimation of the mass transfer. Since the acquisition of enough groundwater for noble gas analysis was not possible in most of the boreholes because of the very low hydraulic conductivities of some Keuper claystones, Osenbrück et al. (1998) used porewater extracted from freshly drilled rock cores.

In building the model for ERAM, the groundwater recharge was estimated by comparison of several common calculation methods; also, a pedological field mapping campaign was undertaken, the surface run-off was determined for estimation of the water balance, and the surface-water quality was monitored to draw salinity and salt load balances (Langkutsch et al. 1998). With these observed data and estimations, a model (incorporating hydrogeological knowledge of 1997) was conducted in 3D (freshwater conditions) and in 2D-vertical (cross-section with variable density; Langkutsch et al. 1998). In regions of the modeled area of Morsleben where the model did not fit the measurements (water levels in observation wells) or showed unrealistic high or low values (drawdown in production wells), the initial parameters (recharge, hydraulic conductivities) were adjusted. Thus, the mean deviation between the water levels of the model and those observed in the wells, which represents the mean error of the model, could be reduced from 2.95 to 1.77 m (Klemenzen et al. 2001).

Argillaceous rocks: the Bure Test Site (France)

The Bure Test Site (Fig. 1c) is located within the Parisian Basin, on the border of the districts Meuse and Haute-Marne in north-eastern France. The test site will not be used as a final repository, but only as an underground research laboratory (URL) for Agence Nationale pour la Gestion des Déchets Radioactifs (The National Radioactive Waste Management Agency; ANDRA 2007). The layout of the facility is designed in accordance with French government policy, which requires a reversible final repository for at least 100–300 years. Thus, future generations should be able to modify the procedure for the repository closure (ANDRA 2006a, 2009).

One of the most important required criteria for deep geological repositories is the proof of no groundwater circulation within the repository (ANDRA 2007). The host rock of the URL is the Callovo-Oxfordian clay, which is surrounded by two aquifers: the Oxfordian limestone on top and the Dogger limestone below (Teles et al. 2007). The marine clay of the Callovo-Oxfordian formation was deposited about 155 million years ago, has a thickness of about 130 m, is regular in shape, provides a remarkable horizontal homogeneity, and shows a very low permeability of about 10^{-6} m a^{-1} . There is only slow and very slight water circulation within the surrounding formations (ANDRA 2007). To exclude the potential of later conflict of interests, a 2,000 m deep borehole was drilled in 2008. By the determined geothermal gradient (66°C in 2,000 m) and its low productivity, a potential future use of the regional aquifers as a geothermal resource could be excluded (ANDRA 2006a). Its permeability is the fundamental physical property of the investigated host rock formation of interest. The groundwater research of ANDRA is focused on the behaviour of pore water and the permeability of the host rock under overburden pressure. The sorption and retention behaviour of the clay is another of the main research interests at the Bure Test Site.

The investigations at Bure started in 1999 with a 3D-seismic survey over 4 km². Afterwards (between 2000 and 2004), scientific drilling programs over an area of about 2,000 km² were conducted to characterize the regional geology, the hydrogeology and the structural features of the Callovo-Oxfordian argillites and of the Dogger limestones (Rebours et al. 2006). During the specific hydrogeological drilling program (2003 and 2004), nine deep boreholes (down to a maximum depth of about 920 m) were constructed (Delay 2006). The hydraulic data related to the argillite were determined by short-term hydraulic packer tests (24–72 h at about 10 regular intervals) and long-term monitoring of formation pressures by electromagnetic pressure gauge (EPG; Distinguin and Lavanchy 2007). For the long-term investigations, about 130 boreholes were equipped with sensors, which record deformation by overburden pressure and the pore-water pressures. The pressure equivalent to a 400-m water column in the overburden limestone and marly rock leads to a strong compaction of the Callovo-Oxfordian argillite and the reduction of its porosity. Because of the lower quantity of contained water in the clay, its mechanical strength is enhanced, compared with argillaceous rock found at the ground surface. The displacement of the walls of a repository structure would amount to less than a few centimetres after 1,000 years (ANDRA 2006b, 2007). The Callovo-Oxfordian formation is overpressured, which can be explained in part by osmotic processes (Gueutin et al. 2007). The stability of the host rock during the excavation of the test site facilities (shaft and drifts) and the according change of the stress field distribution (causing micro-cracking and alteration of the mechanical and hydraulic properties of the host rock) were investigated and modelled (Fabian et al. 2007). The behaviour of hydromechanical stability of argillaceous rock during dissolution, which increases the porosity, was investigated (Haxaire and Djeran-Maigre 2009).

An important transport mechanism of contaminants in argillaceous rocks is mass transfer by diffusion in addition to transport in fractures. Therefore, the main focus of the geochemistry research program at the Bure site is on the behaviour of the interstitial fluids and on the diffusion and retention capabilities of the radionuclides. For determination of diffusion of radionuclides in clay, Cormenzana et al. (2008) conducted laboratory studies on samples from boreholes drilled vertically through the clay bedding. The tracers (tritium and ⁸⁵Sr) were injected into the center of the cylindrical core sample. After a certain time, the core was sampled by drilling small bores in three concentric circles around the center. The so obtained small cores were cut in slices, which were then analyzed for the tracers. By this procedure, the 3D distribution of the tracers could be investigated. By the orthogonal bedding of the cores in these studies, the modeling of transport was simplified. In addition to the scale-dependent uncertainties of laboratory observations, which should deliver conclusions on the field scale, it cannot be ruled out that the used samples were disturbed by the core drilling. Drilling may produce artificial fissures within the argillaceous rock and may affect the observed mass transport. To exclude these

uncertainties, several in-situ diffusion experiments were conducted (Appelo et al. 2008; Samper et al. 2008). The changes of solute concentration within a borehole by reactions and transport between porewater and borehole solution were monitored for 1 year and modeled with the program PHREEQC (used for modeling geochemical reactions and aqueous equilibria; Appelo et al. 2008). By this approach, the in-situ porewater composition can be determined without subsampling from rock samples, which affects the quality of the data with many uncertainties (contact with air, loss of CO₂, change of chemistry by leaching with pure water, and sequential compositional changes during squeezing or centrifuging). Because the equilibrium in the borehole was not reached after 1 year, the authors intended to verify the model-porewater concentrations after some 3–4 years (Appelo et al. 2008).

Samper et al. (2008) pointed out that interpretation of results from in-situ borehole studies was very complicated because of various non-ideal effects. They tried to estimate the influence of these effects on the observed diffusion. It was found that the filter, the gap between filter and borehole wall, and the by the excavation disturbed rock significantly affect diffusion processes between aquifer and borehole and therefore have to be taken into account for interpretation of in-situ borehole studies. In general, for all borehole tests for in-situ determination of parameters (permeability, diffusion) in argillaceous formations, the very long periods (months to years) for re-equilibration of the system, after the disturbances induced by drilling and testing, have to be taken into account (Distinguin and Lavanchy 2007). Though diffusion is probably the most important transport mechanism at the Bure test site, Beaucaire et al. (2008) showed at another site (Tournemire, France) that fracture-related relatively fast groundwater-flow velocities in argillaceous rock are also relevant. Beaucaire et al. (2008) also reported on chemical alterations of fluids in boreholes at that site. Since the boreholes were drilled at Tournemire, reduction of SO₄²⁻ and oxidation of dissolved organic carbon have changed the isotopic composition of the fluids within the surrounding aquifers and influenced the ¹⁴C groundwater ages.

For proof of safety, the impact of the repository on man and the environment was evaluated for the following 1 million years. The probable future development of the land surface was estimated by topographic analysis of the past 2 million years in the region. In those scenarios, the Callovo-Oxfordian clay formation plays a major role for immobilizing, delaying, and limiting the migration of the radionuclides. Currently, the regional groundwater flow system is from the recharge areas in the south and east of the Bure Test Site towards the centre of the Parisian Basin. The general flow direction is expected to undergo relatively few changes. However, the repository disturbs the natural hydraulic equilibrium within the Callovo-Oxfordian. It will need about 100,000 to 200,000 years to establish a new equilibrium (ANDRA 2006b). Some river valleys will reach the Oxfordian limestone aquifer

during that time by erosion. This will probably cause changes in the upper aquifer, but will not strongly impact the host rock during the next million years (Teles et al. 2007). The prospective investigation program (until 2015) includes pore-water characterization, the study of hydrothermal coupled phenomena, and further research on diffusion. This is required for quantifying the safety margins during the modelling of flow-migration of water-gas systems and of reactive migration in a desaturated environment more precisely (Delay 2006).

Conclusions

Deep groundwater research was underrepresented in the hydrogeological sciences for a long time and accordingly little is known about its behaviour. Recently, deep groundwater is not only defined by its depth, but by its genesis, age, chemical composition, etc. (Einsele et al. 1983). It is now widely accepted that deeper aquifers are dynamic systems, which are influenced by both surface processes (from the meteoric cycle) and crustal processes (from the lithosphere). The aim of recent research projects is to present integrated concepts about the past and the future evolution of deep groundwater systems. Questions as to the transport behaviour of deep groundwater and the physical laws of its movement have not been answered so far. This is caused by the lack of interest of the research community in the past, and by the difficult and expensive access to deep aquifers. As shown in the selected case studies, the aims of deep groundwater research studies are fundamentally different from shallower “conventional” projects. Depending on the specific questions, research is directed to aquifers that contain large amounts of hot water, or formations with as little groundwater movement as possible. Deep groundwater research is often challenging: high demands on the technical equipment, highly saline fluids, low permeabilities and low sample volumes. Many well-established methods for hydraulic characterization are not or hardly applicable because of the generally small number of monitoring wells (e.g. tracer tests), slow groundwater velocities (e.g. fluid logging), and low hydraulic conductivities, often combined with local zones of high conductivities from fissures. Some single-well methods for estimation of groundwater flow velocity have been established in the last few years using the dilution characteristics. They promise advances in determination of groundwater velocity and even flow direction. However, these methods may overestimate velocities due to the impact of the borehole on the flow field. Hydrochemical and isotopic characterization of the fluids is often technically limited because of contamination with drilling mud (which is necessary during excavation of boreholes), and very long duration of pumping until the samples are delivered hundreds of meters to some kilometres up to the ground surface (causing degassing, change of temperature, and accordingly change of chemical equilibriums). It seems that, at least in some settings (e.g. argillaceous rocks), the boreholes themselves affect the chemical characteristics of

the fluids within the formation. Another difficulty for most in-situ tests is that processes for reaching equilibrium are very slow at those depths (caused by the low flow velocities). Accordingly, often chemical equilibrium is not reached between drilling and testing or sampling. Additionally, the tests often cannot be conducted before the aquifer reached equilibrium again (which may take years). Although numerical modelling became a fully developed state-of-the-art technology for all kinds of shallow-groundwater projects in the last decade, this method is difficult to apply to deep groundwater systems because of the lack of data and the uncertainties of parameter estimation.

Altogether, both the heterogeneity of the deeper subsurface and the differing goals of research projects lead to very different strategies and methods. The search for final repositories, development of deep geothermal energy techniques, or storage of CO₂ are the driving forces for development of methods for deep groundwater research and therefore for a better understanding of these systems.

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